Project Status Report

High End Computing Capability
Strategic Capabilities Assets Program

August 10, 2017

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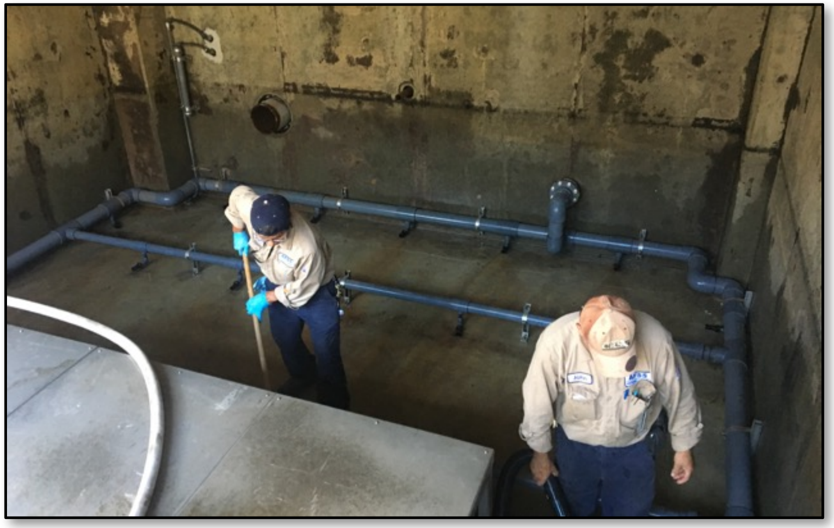
HECC Plans and Successfully Completes Annual Facility Maintenance

- The HECC Facilities team (coordinating with ARC Code J and other HECC groups) successfully completed annual facility maintenance activity for building N258 on July 22 and 23.
- Facilities-related activities included:
  - Cleaned all 4 cooling tower cells, and repaired a bad valve actuator on one of the cells.
  - Cleaned 3 of 4 chillers. The 4th chiller will be cleaned after Chiller #1 is repaired.
  - Successfully attached and removed D-Wave quantum system from temporary cooling and power.
  - Completed moving all PRACA-related infrastructure in N258 to a circuit that was covered by the backup generator. PRACA remained functional throughout the shutdown.
  - Changed all air handler filters.
  - Cleaned and checked all building 480V (and below) circuit breakers.
  - Checked and tested the entire fire alarm and suppression system.
  - Torque-tightened all breakers in the N258/R230 power distribution units, which helped reduce high-resistance overheating.
  - Cleaned the sub-floor of N258/R230.
- All systems returned to operation on schedule, with the exception of Merope, which encountered filesystem issues, but returned to operation by early afternoon the same day.

Mission Impact: Annual facility maintenance helps ensure that all aspects of the highly complex HECC supercomputing facility continue operating at peak efficiency and reliability.



NASA Ames Code J engineers cleaned one of the new N258 cooling tower cells, as part of the annual NAS facility maintenance activities.

POCs: Mark Tangney, mark.l.tangney@nasa.gov, (650) 604-4415, NASA Advanced Supercomputing (NAS) Division;
Chris Buchanan, chris.buchanan@nasa.gov, (650) 604-4308, NAS Division, CSRA LLC

HECC Completes System Maintenance Activities

- Systems engineers successfully completed maintenance activities on HECC resources prior to the annual building shutdown (see slide 2). The activity was timed to coincide with facility maintenance work, in order to minimize the impact on users.
- Activities completed include:
  - Updated firmware.
  - Refreshed infrastructure systems.
  - Applied operating system patches and software updates.
  - Replaced faulty components on the compute and storage subsystems.
  - Ran filesystem integrity checks on Lustre filesystems.
- An upgrade to the cluster management software was postponed due to unexpected issues with the software. This is being worked with the vendor to correct the problems.

Mission Impact: Regular maintenance on the HECC systems provides a stable and well-performing system for NASA users.

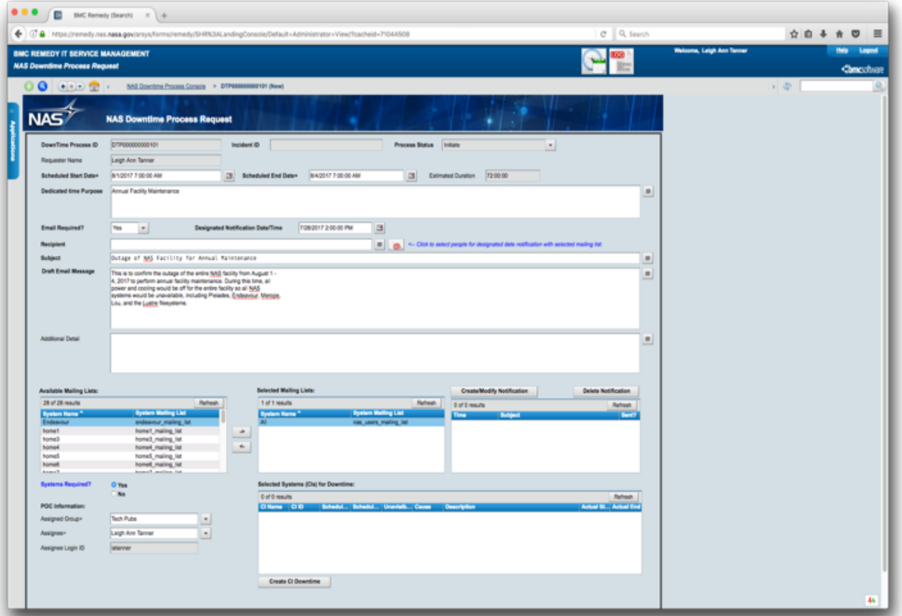
HECC systems maintenance activities were scheduled to coincide with building maintenance work to reduce the impact on users.

POCs: Bob Ciotti, bob.ciotti@nasa.gov, (650) 604-4408, NASA Advanced Supercomputing (NAS) Division;
Davin Chan, davin.chan@nasa.gov, (650) 604-3613, NAS Division, CSRA LLC

Tools Team Develops Remedy Application to Schedule System Downtime and Email Users

- The HECC Tools team developed a Remedy application that helps schedule system dedicated time and sends out email notifications to users.
- Improvements were developed over the past several months and validated through testing by the User Services staff.
- The interface streamlines the complicated process of scheduling downtime for the supercomputing systems, and ensures that users are informed of the downtime.
- Prior to development of the tool, scheduling dedicated time and emailing users were manual processes that sometimes resulted in duplication or missing emails.
- One of the features of the tool is that staff can set action items with dates for when to automatically send out email reminders to users—another task that was done manually in the past.

Mission Impact: With the complexity and timing involved in scheduling dedicated time for HECC systems as well as sending email notifications to users, this new tool eliminates duplication of effort and streamlines the process.



Screenshot of the Remedy application setting up dedicated time for Pleiades and sending out email to all Pleiades users.

POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, CSRA LLC

This Year's Annual Contingency Plan Test Based on Real Power Outage

- NAS Division staff successfully completed the required annual contingency test.
- This year's test was based on an actual power failure that affected the Ames Research Center campus in February 2017.
- Each HECC/NAS support group reported:
  - How they responded to this event back in February.
  - A retrospective assessment of how they could have improved their response.
  - Lessons learned from this event, and the identification of any changes that should be made to the NAS Contingency Plan.
- When power was restored in a few hours:
  - Our personnel worked efficiently to get HECC systems back into operation.
  - The whole situation was rectified in sufficient time that it did not trigger the NAS Contingency Plan's "heavy duty" response.
  - No changes needed to be made to the NAS Contingency Plan.

Mission Impact: Successful completion of NASA's annual contingency plan test helps the HECC project maintain its authorization to operate agency supercomputing resources

Test Based On Real Power Outage

Supercomputers, storage and support systems down

NAS staff responded and restored all systems when power was restored

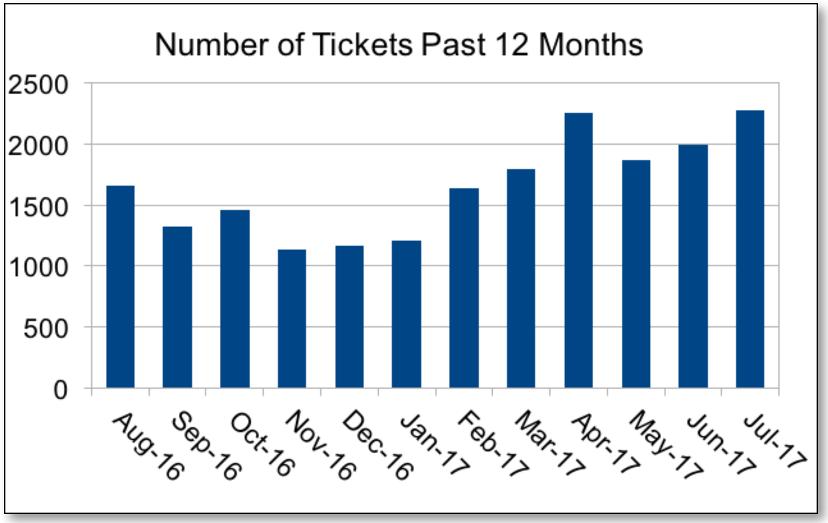
This year's NAS contingency test was based on an actual power outage that occurred in February 2017.

POC: Thomas. H. Hinke, thomas.h.hinke@nasa,gov, (650) 279-4053, NASA Advanced Supercomputing Division

HECC Support Staff Continue Providing Important Assistance to Users

- During the past 12 months, HECC staff provided support to 1,200 users from all of NASA's mission directorates.
- Support staff across the HECC project processed, tracked, and resolved just under 20,000 tickets for the 12 months from August 1, 2016 through July 31, 2017.
- Staff handled tickets on a wide range of topics—covering automated notification of system issues and resolving a variety of issues for users calling for help. Examples include:
  - Helped users resolve any problems in connection to Pleiades.
  - Modified and improved users' environment settings on their desktop machines, as well as on the HECC resources, to improve their experience.
  - Proactively detected when jobs weren't running, then contacted users to assist with job modifications within minutes of the original job's submission.
  - Continually modified allocations and account expiration dates.
  - Modified quotas to allow users to run jobs that are more disk space intensive.

Mission Impact: Our 24x7 support services staff resolve a wide range of user and systems problems, helping enable users to focus on their mission projects.



HECC support staff resolved 19,770 tickets over the past 12 months.

POC: Leigh Ann Tanner, leighann.tanner@nasa.gov, (650) 604-4468, NASA Advanced Supercomputing Division, CSRA LLC

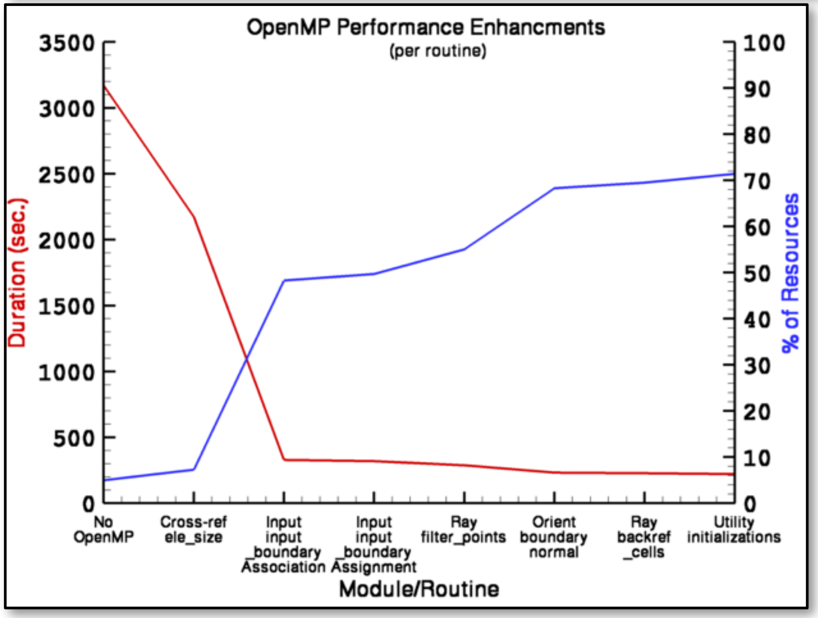
Improving Performance of Ray-Tracing Through Unstructured Meshes

- HECC application experts teamed with aerospace engineer Steve Alter (NASA Langley) to improve performance of his new ray-tracing software, RADIANT, developed to determine the radiative intensity in hypersonic flow fields.
- To obtain the performance improvement, OpenMP was chosen for multithreading, which avoids extensive rewriting of the code.
- APP team members provided guidance and assistance on adding OpenMP directives, and helped debug the parallel version of the code.
- To avoid race conditions when running on multiple threads, it was very important to declare data as private when necessary. See example code:

```
!$omp parallel do shared(npt,xv,yv,zv,xroot,yroot,zroot, &
!$omp                    xyzray,storept,nodlen,tmpcyln) &
!$omp private(ipt,point,xvec,yvec,zvec,dotprod,ds)
      do ipt=1,npt
         point(1) = xv(ipt) - xroot
         point(2) = yv(ipt) - yroot
         point(3) = zv(ipt) - zroot
         call cross_product_by_vector(xyzray,point,0,xvec,yvec,zvec)
         dotprod = dot_product(xyzray,point)
         ds = sqrt(xvec*xvec + yvec*yvec + zvec*zvec)
         if (ds <= nodlen(ipt)) then
            tmpcyln(ipt) = ipt*sign(1.0_wp,dotprod)
         endif
      enddo
!$omp end parallel do
```

- Employing 20 threads on a 24-core Haswell node showed a 72% usage of resources. The OpenMP parallelization resulted in a 14x speed-up over single-threaded execution.

Mission Impact: Utilizing the Application Performance & Productivity team's expertise, software improvements to RADIANT now enable rapid line-of-sight radiative intensity assessments for hypersonic reentry simulations utilizing unstructured meshes.



Graph showing the parallel efficiency of various routines, when employing 20 threads on a 24-core Haswell node on the Pleiades supercomputer.

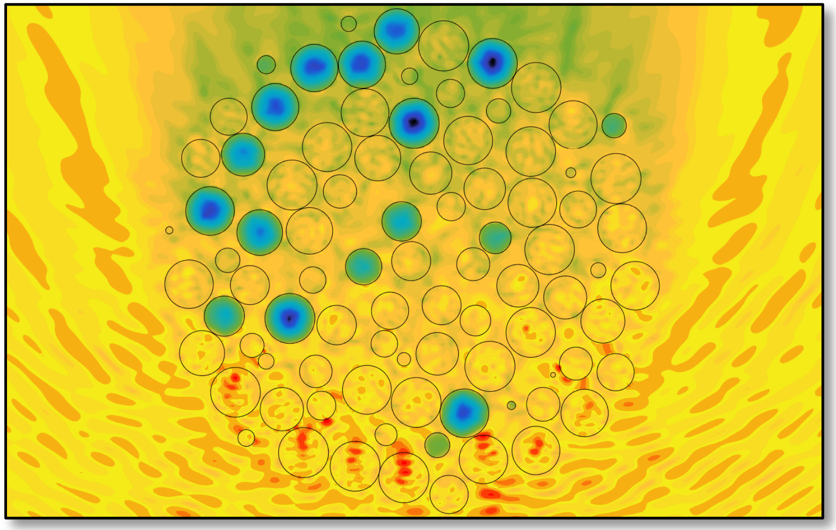
POCs: Stephen Alter, stephen.j.alter@nasa.gov, (757) 864-7771, NASA Langley Research Center; Gabriele Jost, gabriele.jost@nasa.gov, NASA Advanced Supercomputing Division, Supersmith

Modeling Nanoscale Light Scattering by the Lunar Regolith

- The moon's soil (lunar regolith) reflects less light at shorter wavelengths than at longer wavelengths—a result of a set of processes known as "space weathering" that affects materials on the surface of planets and other objects in the solar system.
- To learn the cause of space weathering and understand the optics and physics behind it, researchers are running simulations on Pleiades using the Multiple Sphere T-Matrix Model (MSTM).
  - A combination of laboratory observations and computer models are used to characterize the optical effects of space weathering, with the goal of producing a physics-based computer model that accurately reproduces the observed spectra of objects in the solar system.
  - By helping scientists understand how space weathering affects the spectrum, results will help them identify the composition of the moon, asteroids, comets, & planets.
  - Simulation results are also leading to a better understanding of the role of Mie scattering, which occurs when the particle that scatters the light and the light's wavelength are approximately the same size.
- Future work will increase the complexity of the particles to obtain even more realistic simulations of complex lunar and asteroid compositions.

** HECC provided supercomputing resources and services in support of this work.*

Mission Impact: Researchers supporting NASA missions use HECC resources to vastly reduce computation times. Multiple Sphere T-Matrix Model runs that take 6 – 8 hours on Pleiades would take years to run on a regular desktop computer. Results will help NASA identify the composition of the moon, planets, comets, and asteroids in the solar system.



Visualization of the magnitude of the modeled electric field within a cluster of silica glass and iron particles under illumination by 700-nanometer wavelength light. Dark areas correspond to iron particles that strongly absorb light. Each individual sphere is 1 micron in diameter.

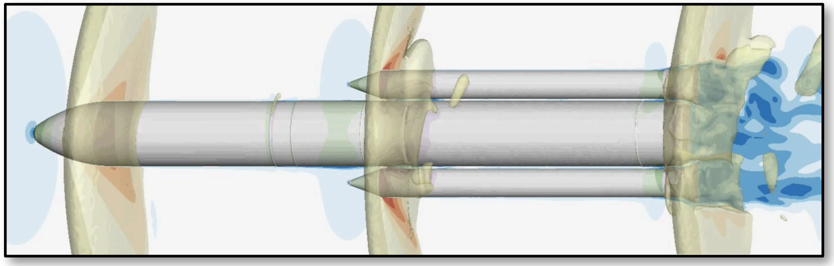
POCs: Carey Leggett, carey.legett@stonybrook.edu; Timothy Glotch, (631) 632-1168, timothy.glotch@stonybrook.edu; Stony Brook University

Improving Prediction of Buffet Forces for Design of the Space Launch System

- As the SLS design matures, the shuttle-based solid rocket boosters (SRBs) may be replaced with advanced boosters of different shapes and sizes than the SRBs.
- CFD experts at NASA Langley (LaRC) have produced simulations to assess the aerodynamic impact of alternate SRB designs, with a focus on predicting the unsteady flow field that causes buffeting.
  - Researchers simulated the transonic flow field about SLS cargo configurations using the FUN3D CFD solver at wind tunnel conditions.
  - Their CFD-based aeroacoustic and buffet data were found to be in excellent quantitative agreement with ground-based test data.
  - Detailed spatial resolution led to greatly enhanced understanding of loads generated by surface pressure fluctuations on the SLS.
- Each simulation typically used 12,000 cores of supercomputing resources and required approximately 36 million core-hours.

** HECC provided supercomputing resources and services in support of this work.*

Mission Impact: Complex flow field simulations for predicting structural dynamic response on SLS cargo configuration designs require the availability of large amounts of HECC supercomputing resources.



This video shows the unsteady transonic flow field about the Space Launch System cargo configuration at mild angle of attack and sideslip. Mach contours (horizontal swaths) are shown on the vehicle symmetry plane. Sonic iso-surfaces are shown in tan.

POCs: Craig L. Streett, craig.l.streett@nasa.gov, (757) 864-2230, William Jones, w.t.jones@nasa.gov, (757) 864-5318), NASA Langley Research Center

HECC Facility Hosts Several Visitors and Tours in July 2017

- HECC hosted 17 tour groups in July; guests learned about the agency-wide missions being supported by HECC assets and some groups also viewed the D-Wave 2X quantum system. Visitors this month include:
  - The Honorable Joe Hockey, Ambassador of the Commonwealth of Australia to the United States; and Frances van Ruth, Trade and Investment Commissioner, Australian Consulate-General.
  - Lieutenant General Michael Shields, Director of the Joint Improvised-Threat Defeat Organization.
  - Scott Robinson, NASA Director of Facilities and Real Estate Division; and Jennifer Groman, NASA Chief of Facilities Engineering Branch.
  - 20 members of foreign consulates in San Francisco toured Ames facilities, including the NAS facility.
  - 150 participants in various NASA summer programs including: Ames interns; students in the Stanford Summer High Performance Computing program; postdocs in the planetary science and data science fields attending the Frontier Development Laboratory program; and K-12 teachers—all received HECC overviews and tours.

Chris Buchanan, HECC networking, security, and facilities lead, gives a tour of the NAS facility's computer room and an overview of HECC capabilities to students from the Stanford HPC program.

POC: Gina Morello, gina.f.morello@nasa.gov (650) 604-4462, NASA Advanced Supercomputing Division

Papers

- "**Foreshock Wave Interaction with the Magnetopause: Signatures of Mode Conversion**," F. Shi, L. Cheng, Y. Lin, X. Wang, Journal of Geophysical Research: Space Physics, July 3, 2017. *
  http://onlinelibrary.wiley.com/doi/10.1002/2016JA023114/full
- **AIAA Propulsion and Energy Forum**, Atlanta, GA, July 10-12, 2017.
  – "**Comparisons Between NO PLIF Imaging and CFD Simulations of Mixing Flowfields for High-Speed Fuel Injectors**," T. Drozda, K. Cabell, A. Ziltz, et al. *
  https://arc.aiaa.org/doi/pdfplus/10.2514/6.2017-4647
  – "**Computational Study of Combustor-Turbine Interactions**," K. Miki, J. Moder, M.-S. Liou. *
  https://arc.aiaa.org/doi/pdf/10.2514/6.2017-4824
  – "**A Flamelet Model with Heat-Loss Effects for Predicting Wall-Heat Transfer in Rocket Engines**," P. Ma, H. Wu, M. Ihme, J.-P. Hickey. *
  https://arc.aiaa.org/doi/pdfplus/10.2514/6.2017-4856
  – "**Phase Separation Analysis in Supercritical Injection using Large-Eddy Simulation and Vapor-Liquid Equilibrium**," D. Banuti, P. Ma, M. Ihme. *
  https://arc.aiaa.org/doi/pdf/10.2514/6.2017-4764
- "**Probing the Dependence of the Intergalactic Medium on Large Scale Environment Using the Low Redshift Lyman Alpha Forest**," S. Tonnesen, B. Smith, J. Kollmeier, R. Cen, arXiv:1707.03409 [astro-ph.CO], July 11, 2017. *
  https://arxiv.org/abs/1707.03409

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Impact of Cosmic Ray Transport on Galactic Winds**," R. Farber, M. Ruszkowski, H.-Y. Yang, E. Zweibel, arXiv:1707.04579 [astro-ph.HE], July 14, 2017. *
https://arxiv.org/abs/1707.04579
- "**Time-Accurate Coupling of Three-Degree-of-Freedom Parachute System with Navier-Stokes Equations**," G. Guruswamy, Journal of Spacecraft and Rockets, July 18, 2017. *
https://arc.aiaa.org/doi/full/10.2514/1.A33835
- "**2010 August 1-2 Sympathetic Eruptions: II. Magnetic Topology of the MHD Background Field**," V. Titov, et al., arXiv:1707.07773 [astro-ph.SR], July 24, 2017. *
https://arxiv.org/abs/1707.07773
- "**Coronal Heating Topology: The Interplay of Current Sheet and Magnetic Field Lines**," A. Rappazzo, et al., The Astrophysical Journal, vol. 844, no. 1, July 25, 2017. *
http://iopscience.iop.org/article/10.3847/1538-4357/aa79f2
- "**The Effects of Inhomogeneous Proton-α Drifts on the Heating of the Solar Wind**," L. Ofman, et al., Journal of Geophysical Research: Space Physics, June 1, 2017 (not previously reported). *
http://onlinelibrary.wiley.com/doi/10.1002/2016JA023705/abstract
- "**Growth and Nonlinear Saturation of Electromagnetic Ion Cyclotron Waves in Multi-Ion Species Magnetospheric Plasma**," L. Ofman, et al., Journal of Geophysical Research: Space Physics, June 29, 2017 (not previously reported). *
http://onlinelibrary.wiley.com/doi/10.1002/2017JA024172/full

** HECC provided supercomputing resources and services in support of this work*

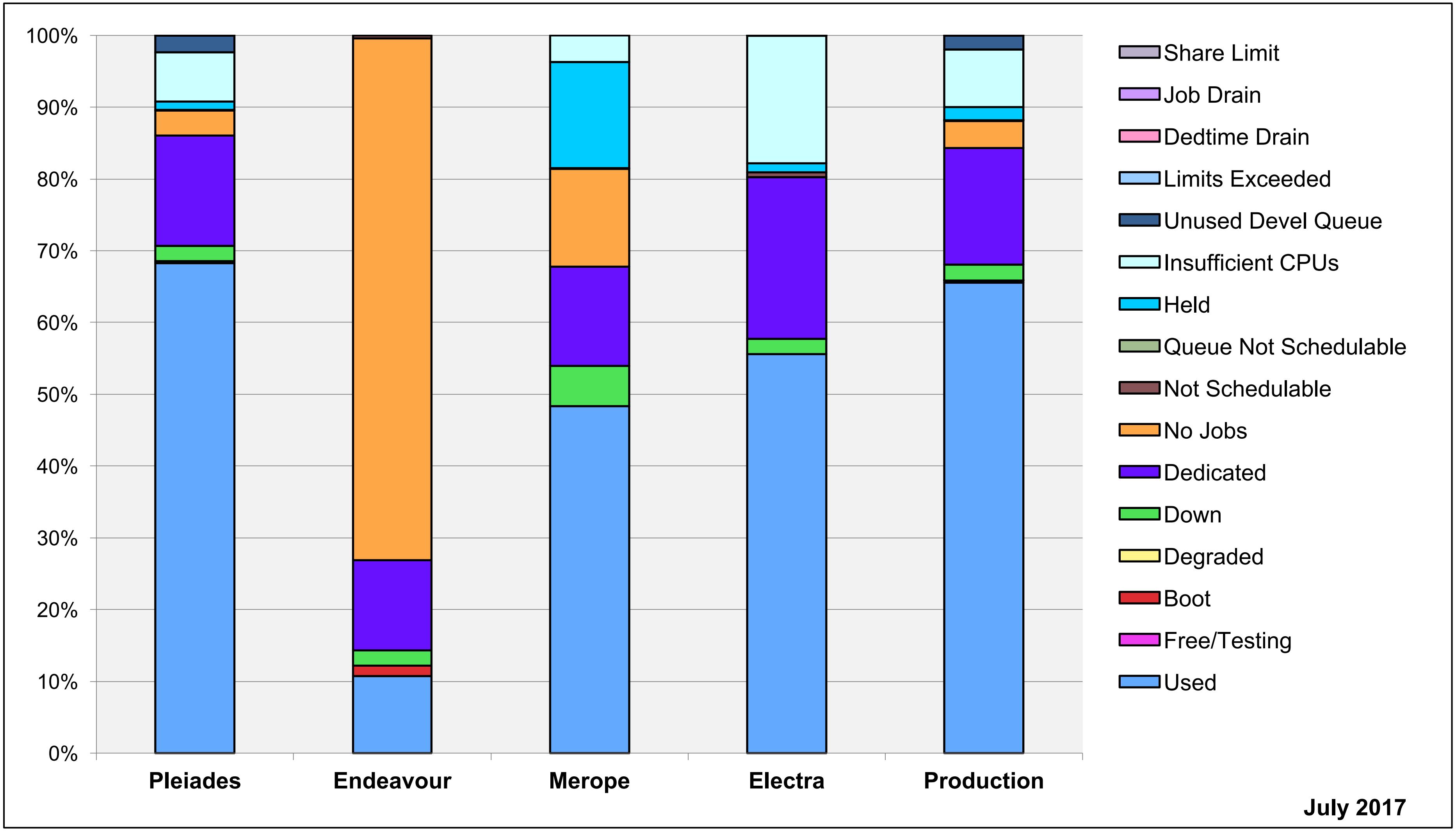
Presentations

- **Solar Heliospheric & Interplanetary Environment Conference**, Quebec, Canada, July 24-28, 2017.
  - "**Realistic 3D radiative modeling of turbulent structure of moderate-mass stars and Sun**," I. Kitiashvili, A. Kosovichev, A. Wray, N. Mansour.
  - "**Using Data Assimilation Methods for Prediction of Solar Activity**," I. Kitiashvili, N. Collins.

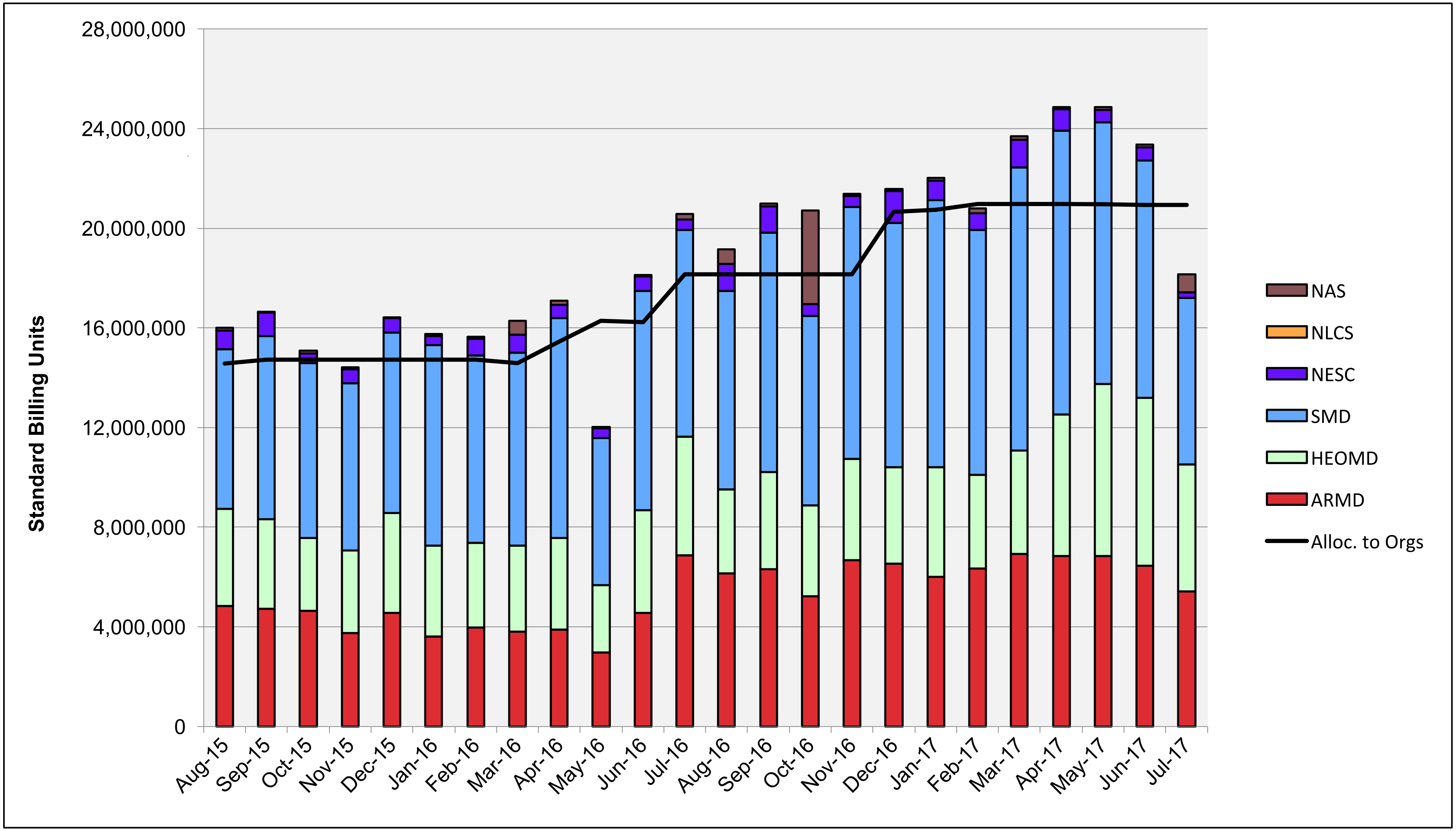
News and Events

- **NASA Using Supercomputers and 3D Modelling to Simulate Asteroid Impact Scenarios**, International Business Times, July 3, 2017. To prevent and prepare for future calamities, Nasa's scientists are using the Pleiades supercomputer and 3D computer-aided design (CAD) software to model and test out the impact of asteroids hitting the Earth. (Covering July 29 original NAS feature, “NASA Researchers Rock the World of Asteroid Simulation.”)
  http://www.ibtimes.co.uk/nasa-using-supercomputers-3d-modelling-simulate-asteroid-impact-scenarios-1628788
- **Mountain View Technology Showcase (Tech Day)**, Mountain View, CA, July 12, 2017—The NASA Advanced Supercomputing Division participated in a booth at the 2017 Mountain View Tech Day, as part of NASA Ames Research Center’s local outreach efforts. Staff members spoke with event attendees about supercomputing at NASA and the division’s ties to Silicon Valley history and industry.
  http://chambermv.org/technology-showcase
- **NASA Captures Sunspot That’s Larger Than Earth: What Are Sunspots And How Do They Form?**, Tech Times, July 14, 2017—A science article on a sunspot imaged by the Solar Dynamics Observatory cites numerical models used to simulate sunspot formation that were run on Pleiades.
  http://www.techtimes.com/articles/211555/20170714/nasa-captures-one-that-s-larger-than-earth-what-are-sunspots-and-how-are-they-produced.htm
- **Is There a Giant Planet Lurking Beyond Pluto?** *IEEE Spectrum*, July 31, 2017—A race is on to discover Planet Nine using astronomy and new computational techniques, including work being done using Pleiades by researchers from the Southwest Research Institute in Colorado.
  http://spectrum.ieee.org/aerospace/satellites/is-there-a-giant-planet-lurking-beyond-pluto

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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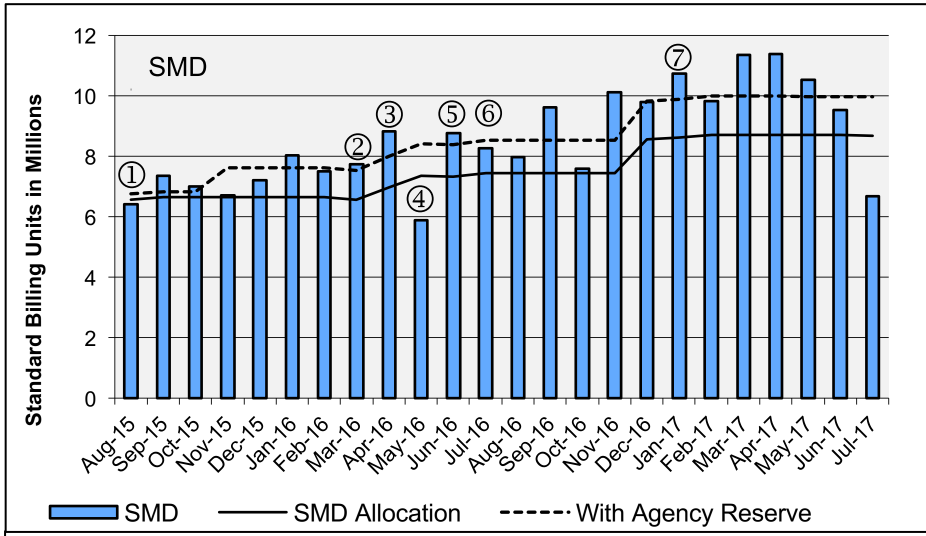
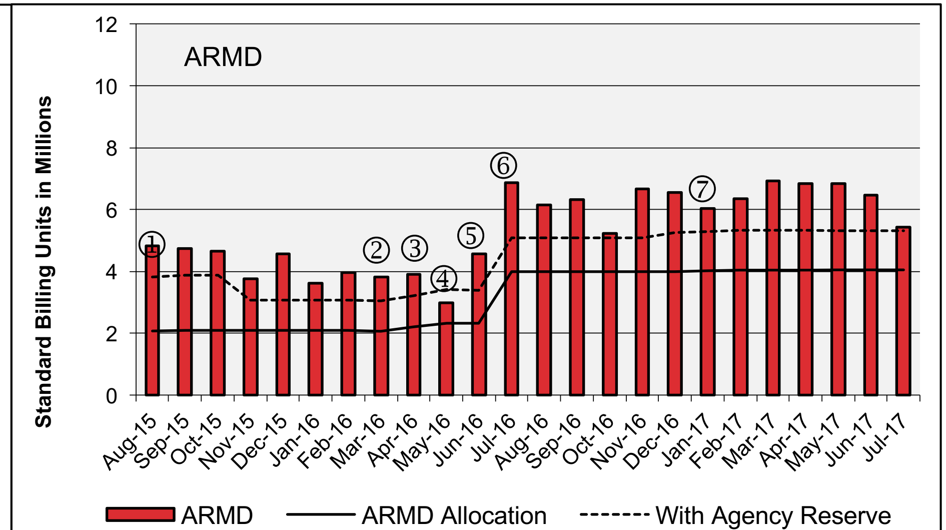
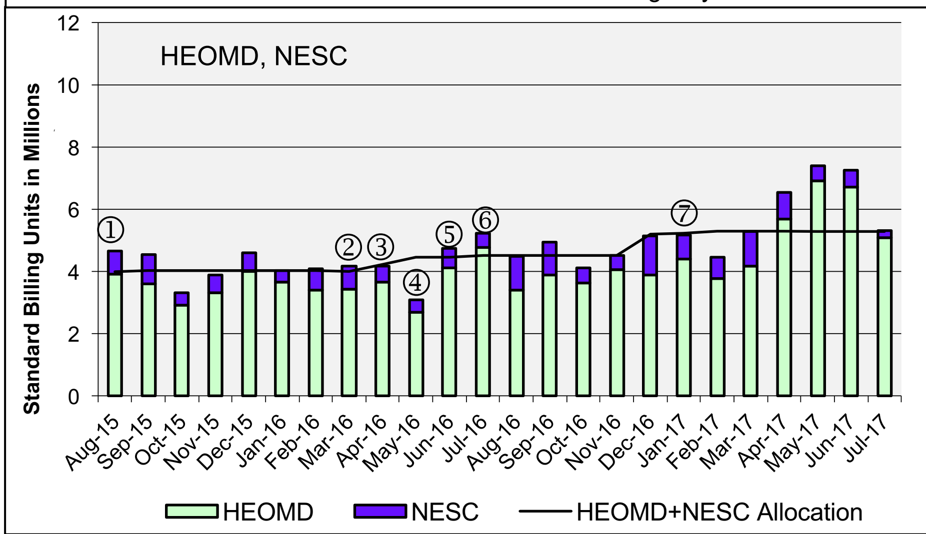
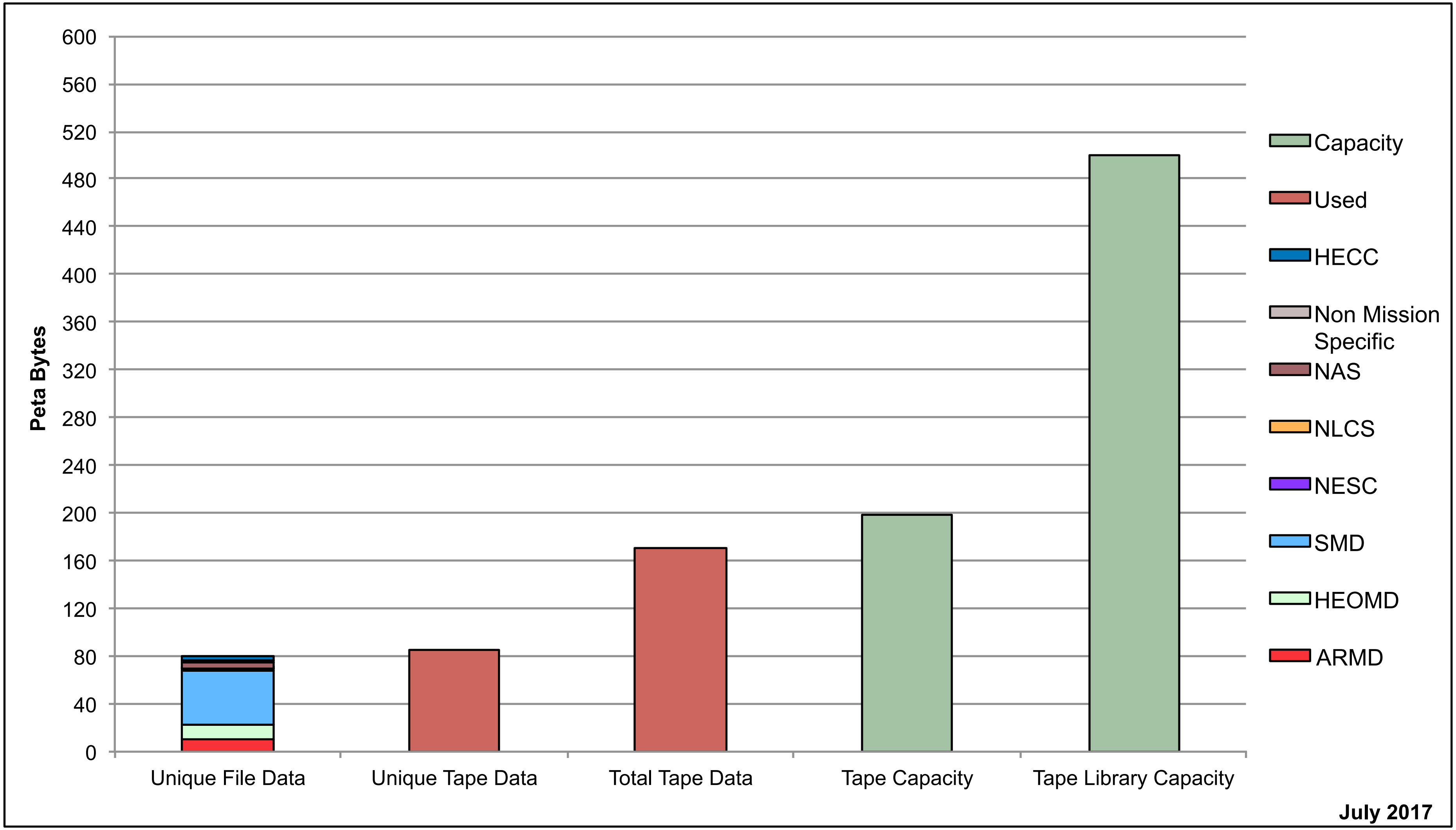






① 7 Westmere ½ racks added to Merope
② 16 Westmere racks retired from Pleiades
③ 10 Broadwell racks added to Pleiades
④ 4 Broadwell racks added to Pleiades
⑤ 14 (All) Westmere racks retired from Pleiades
⑥ 14 Broadwell Racks added to Pleiades
⑦ 16 Electra Broadwell Racks in Production, 20 Westmere 1/2 racks added to Merope

Tape Archive Status



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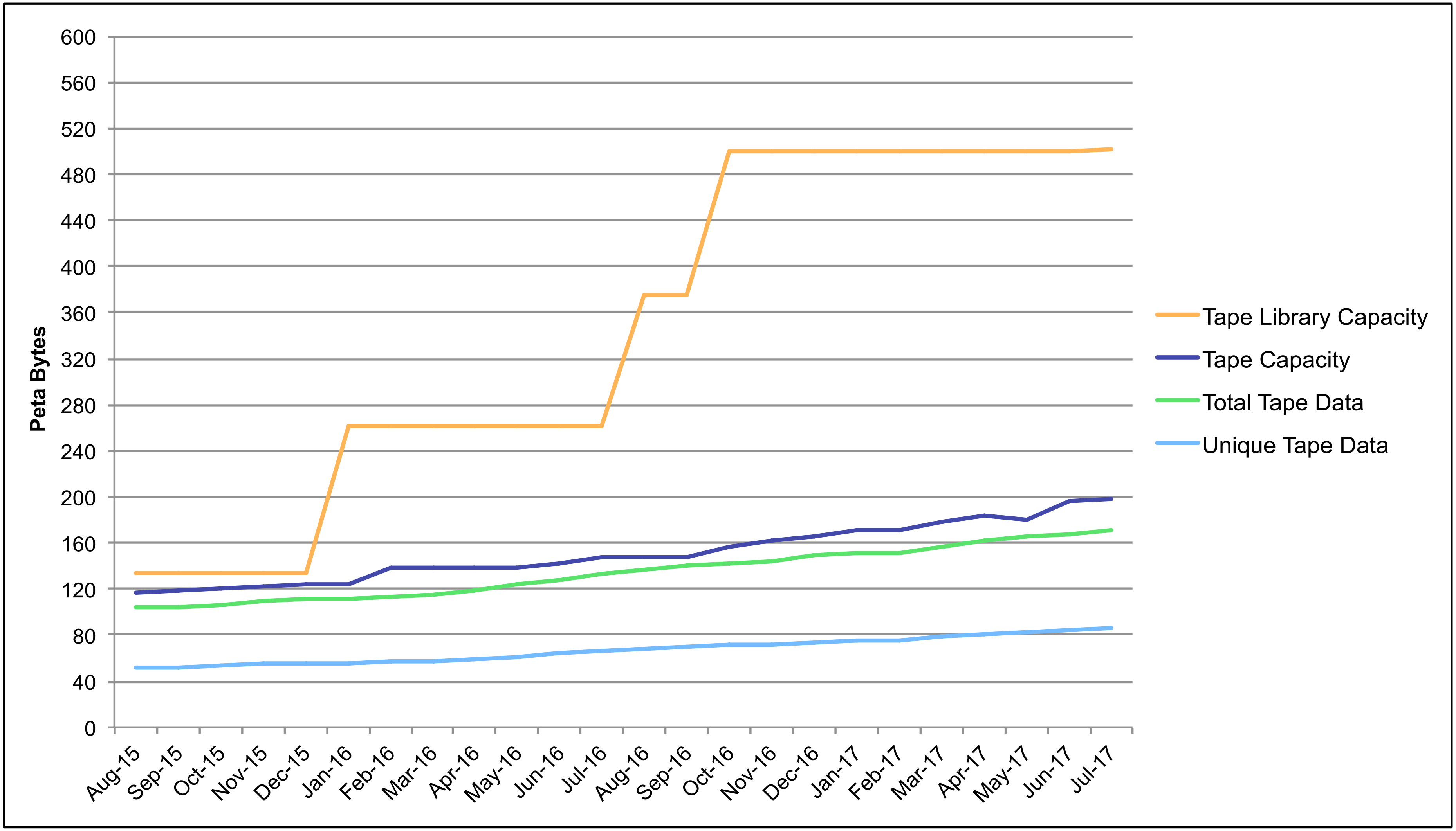
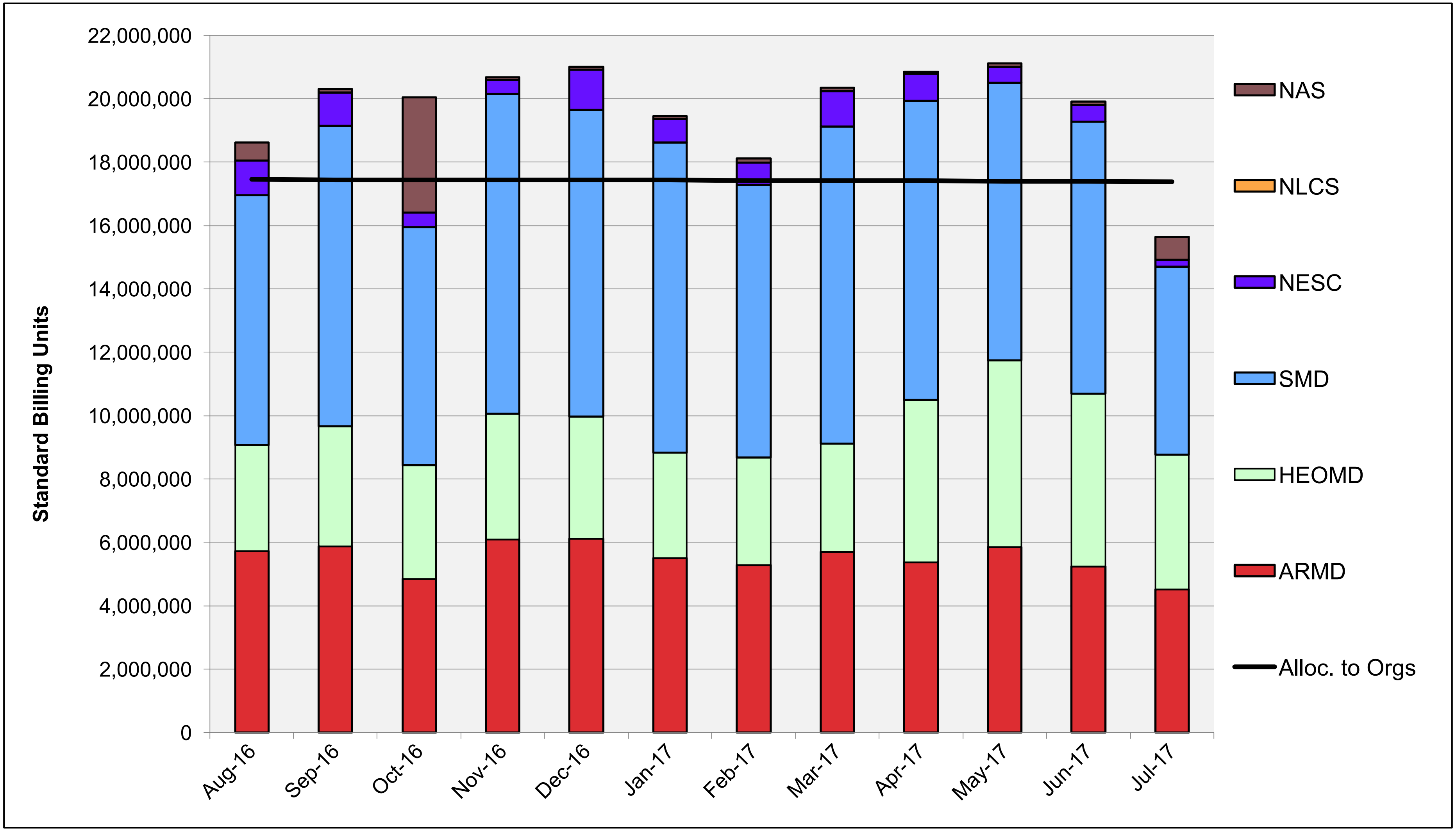
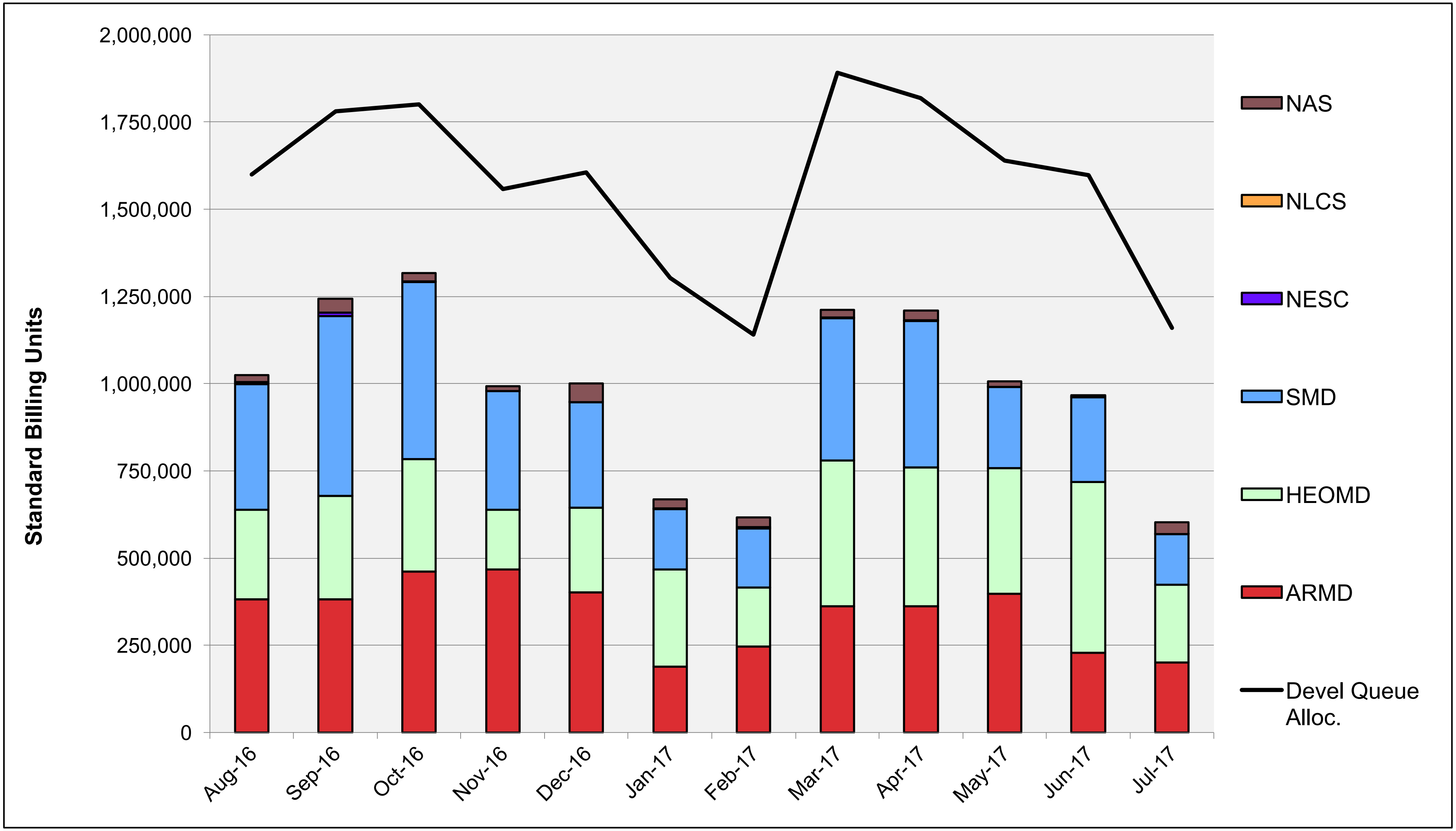


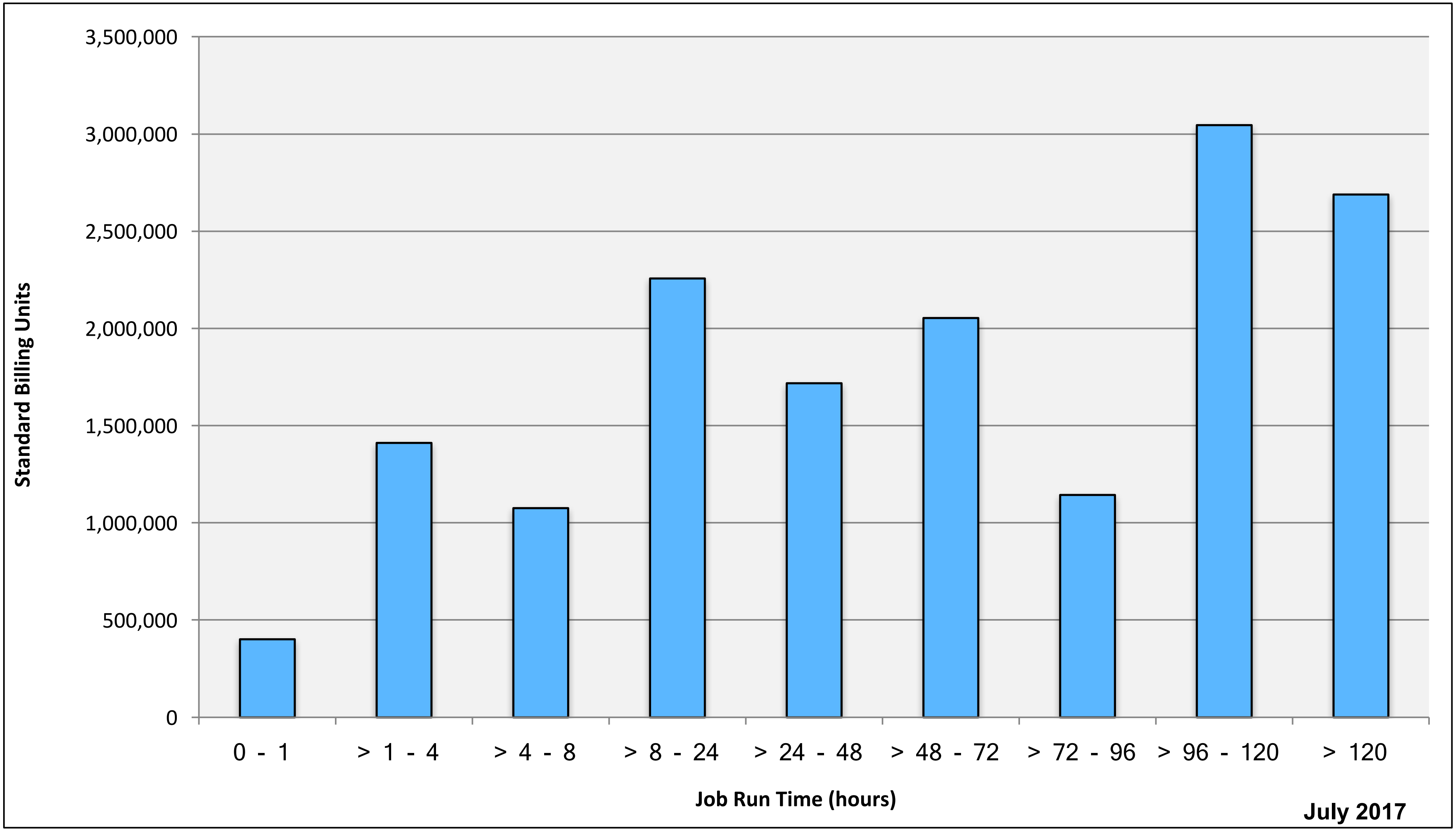
Pleiades: SBUs Reported, Normalized to 30-Day Month



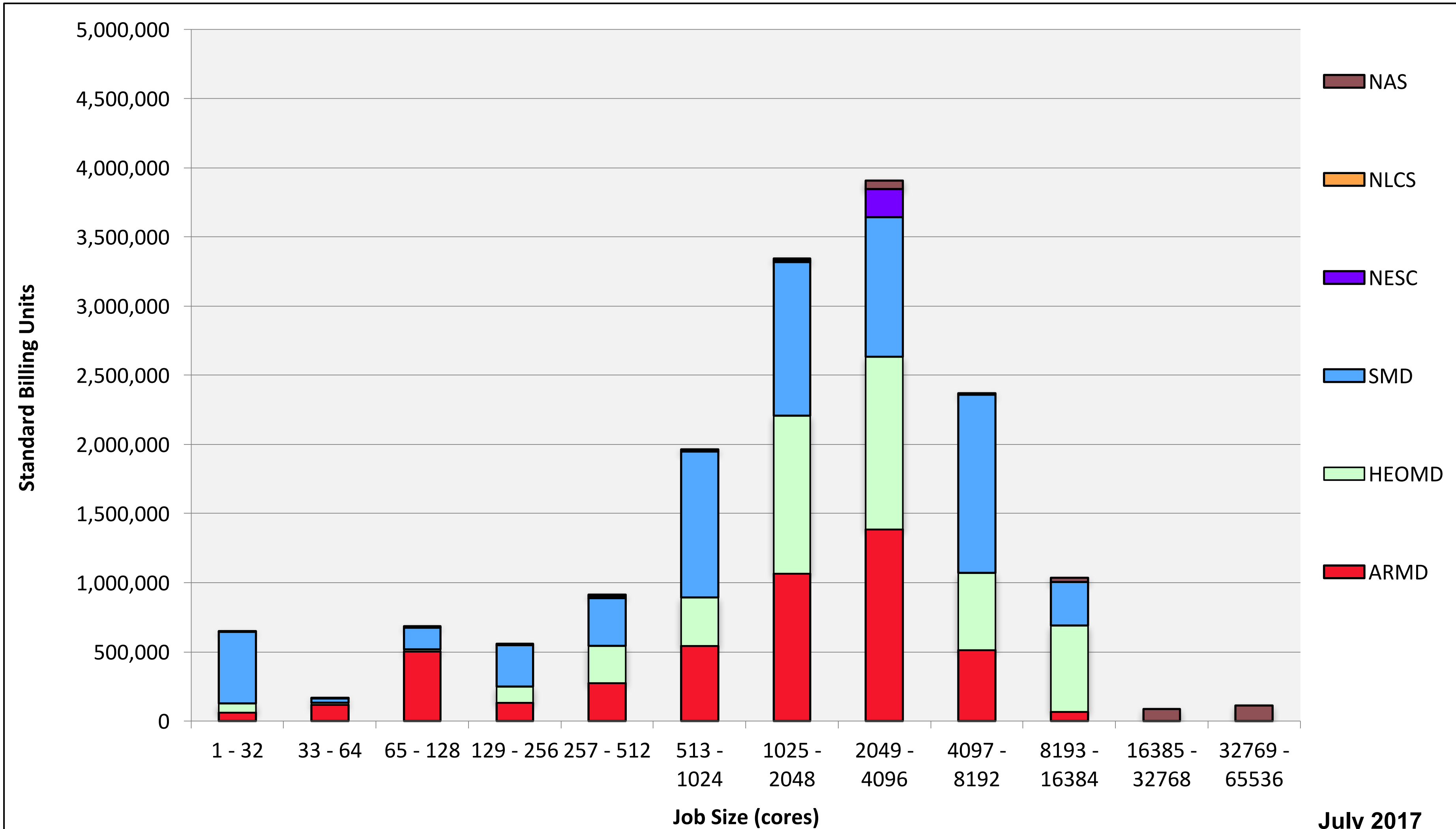
Pleiades:
Devel Queue Utilization



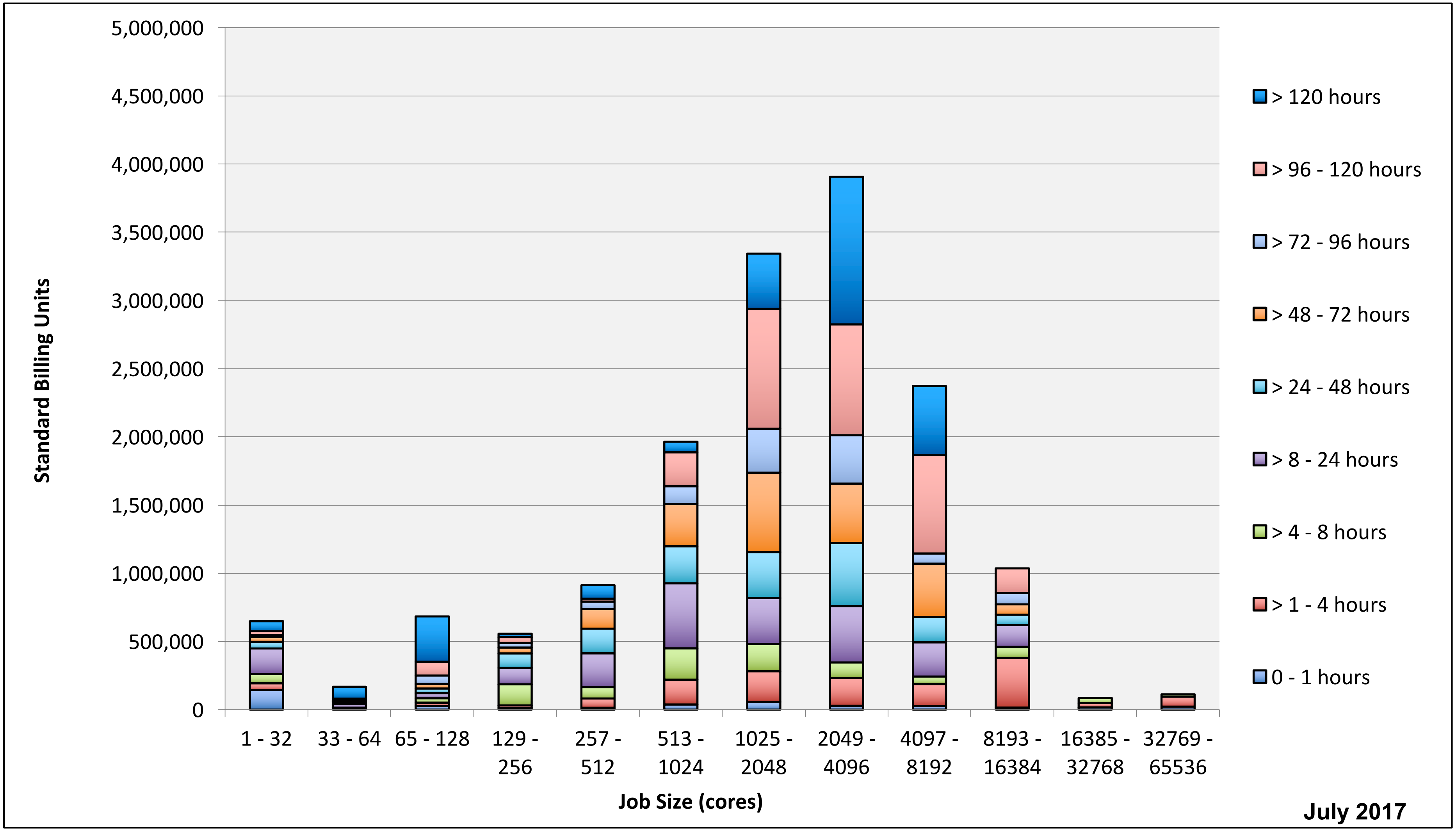
Pleiades: Monthly Utilization by Job Length



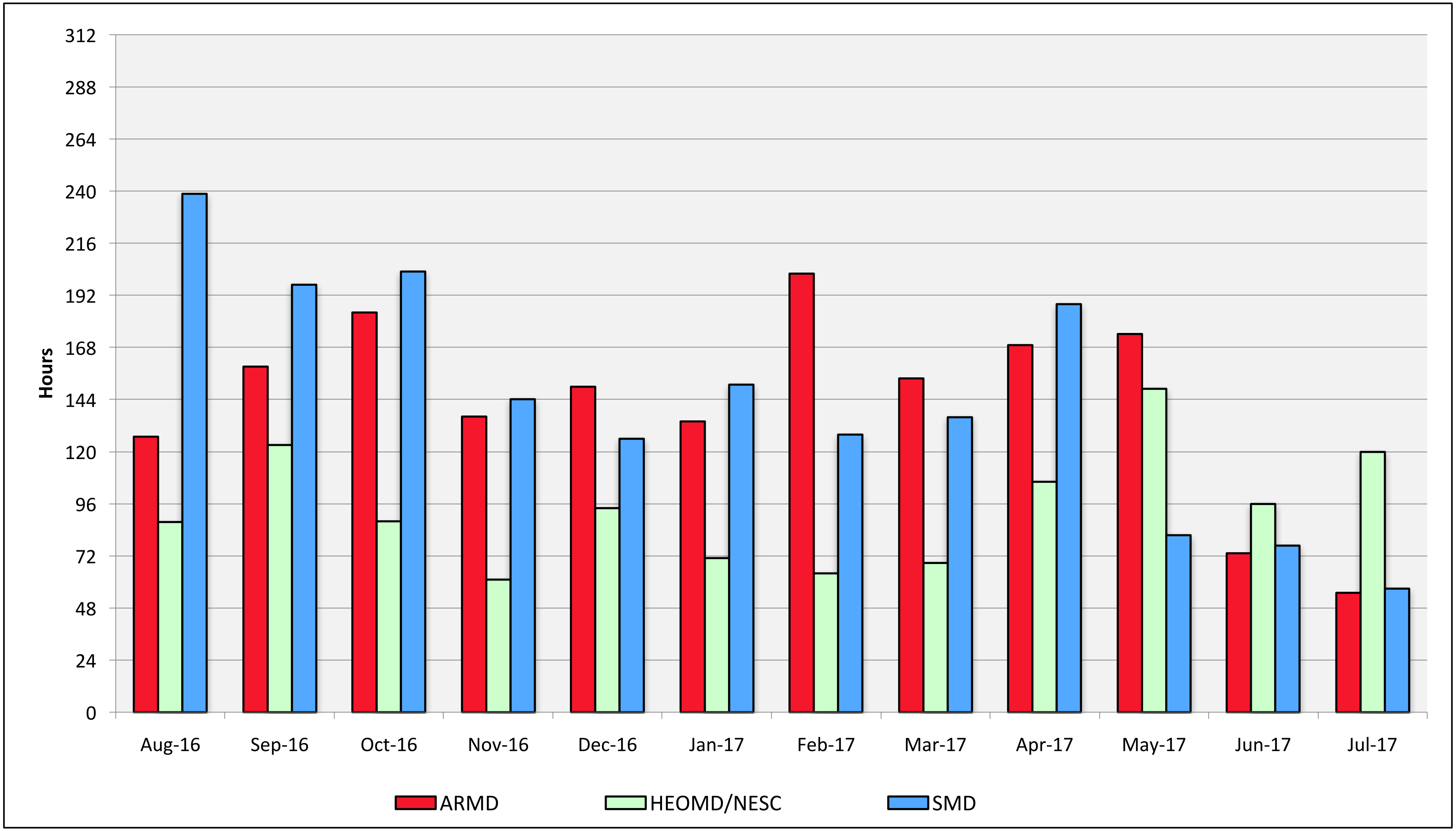
Pleiades: Monthly Utilization by Size and Mission



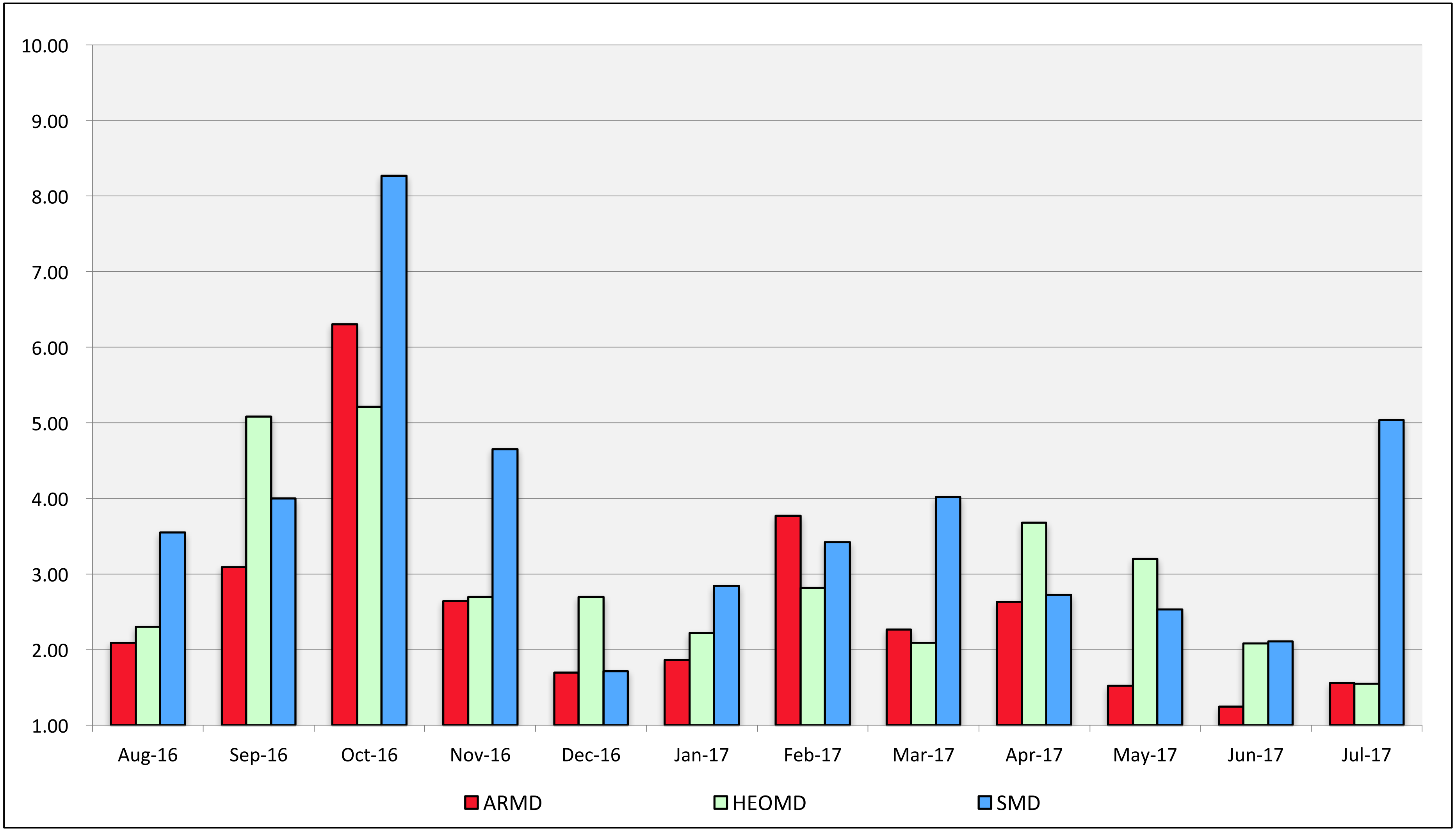
Pleiades: Monthly Utilization by Size and Length



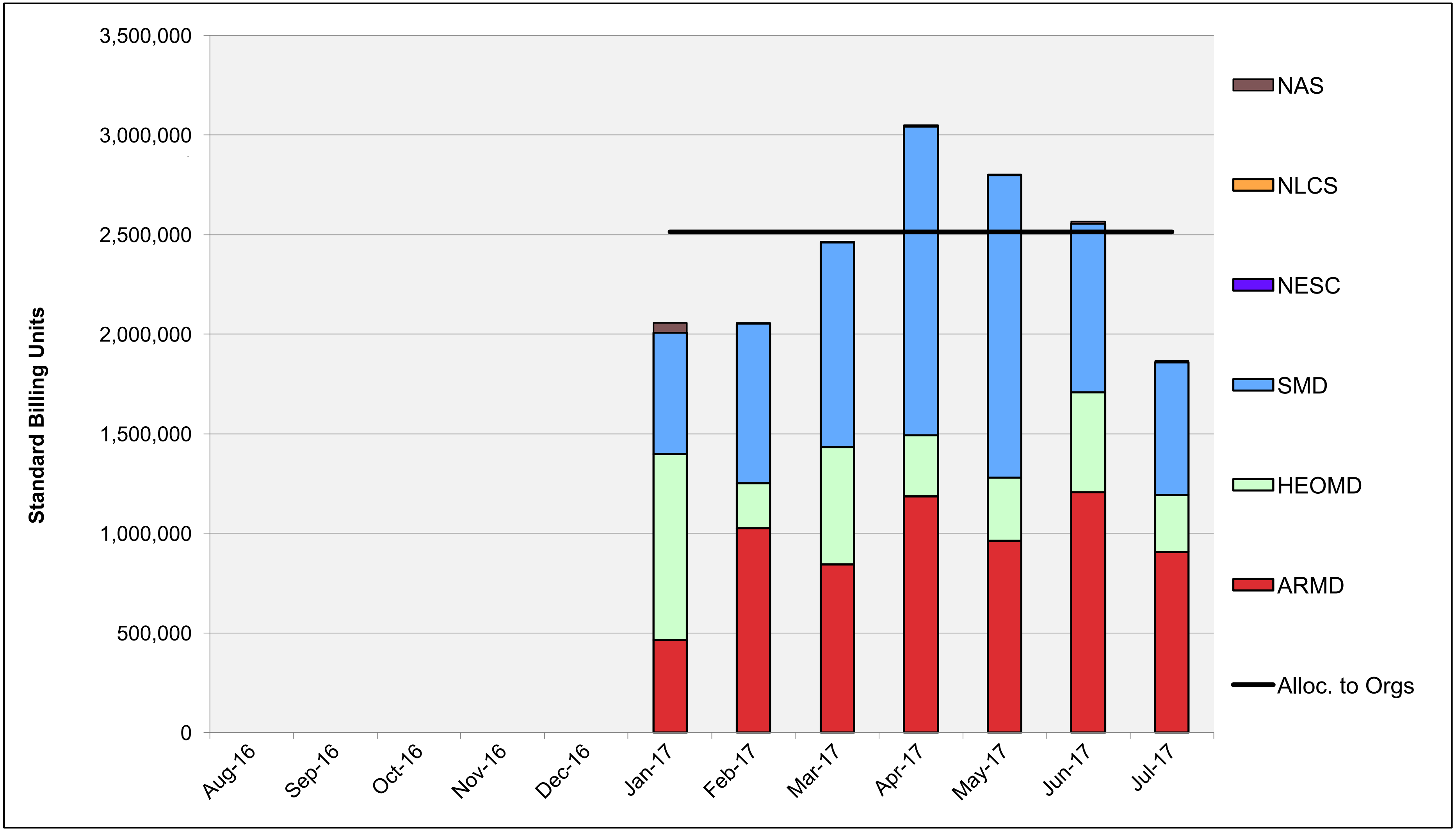
Pleiades:
Average Time to Clear All Jobs



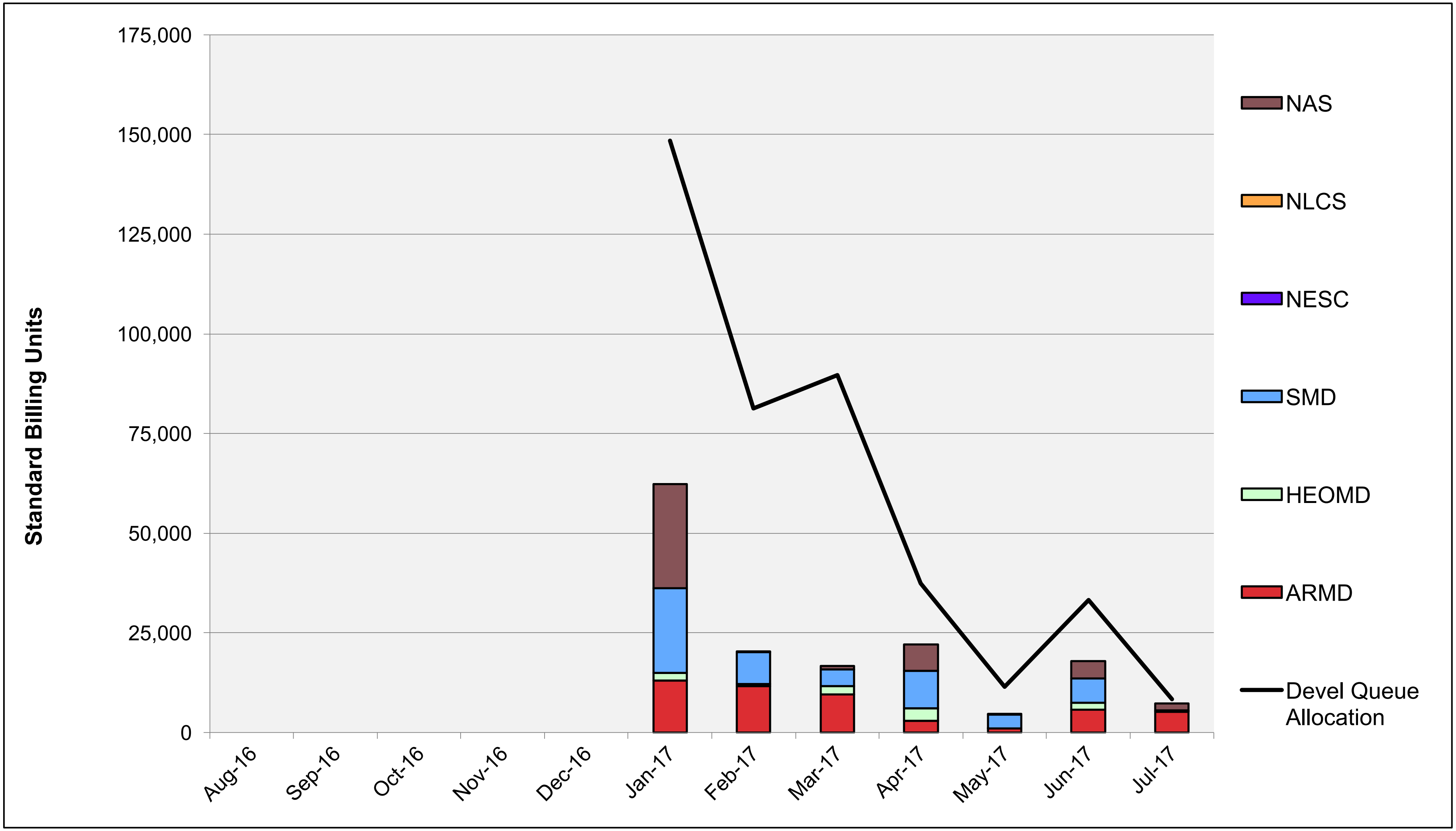
Pleiades:
Average Expansion Factor



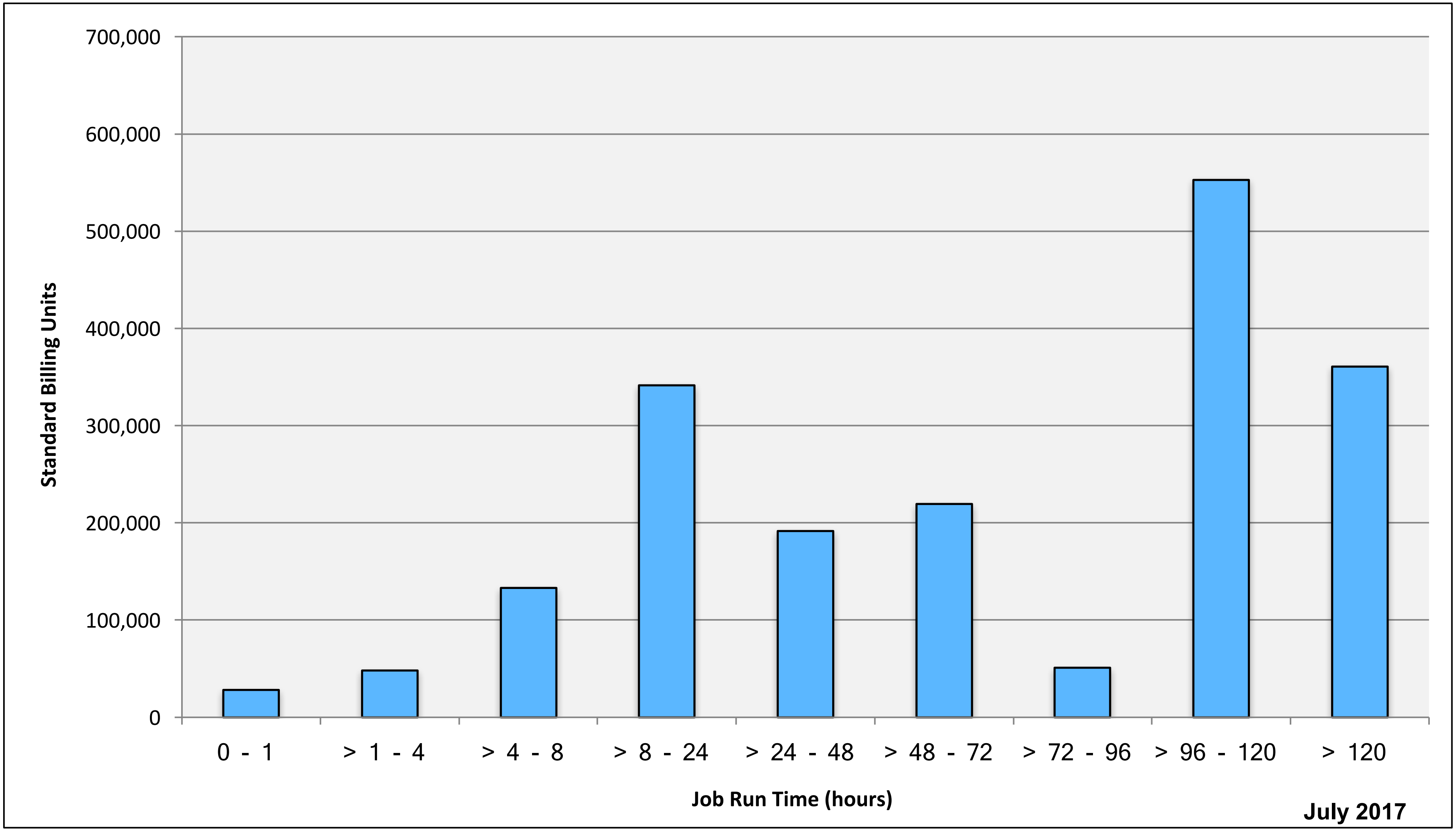
Electra:
SBUs Reported, Normalized to 30-Day Month



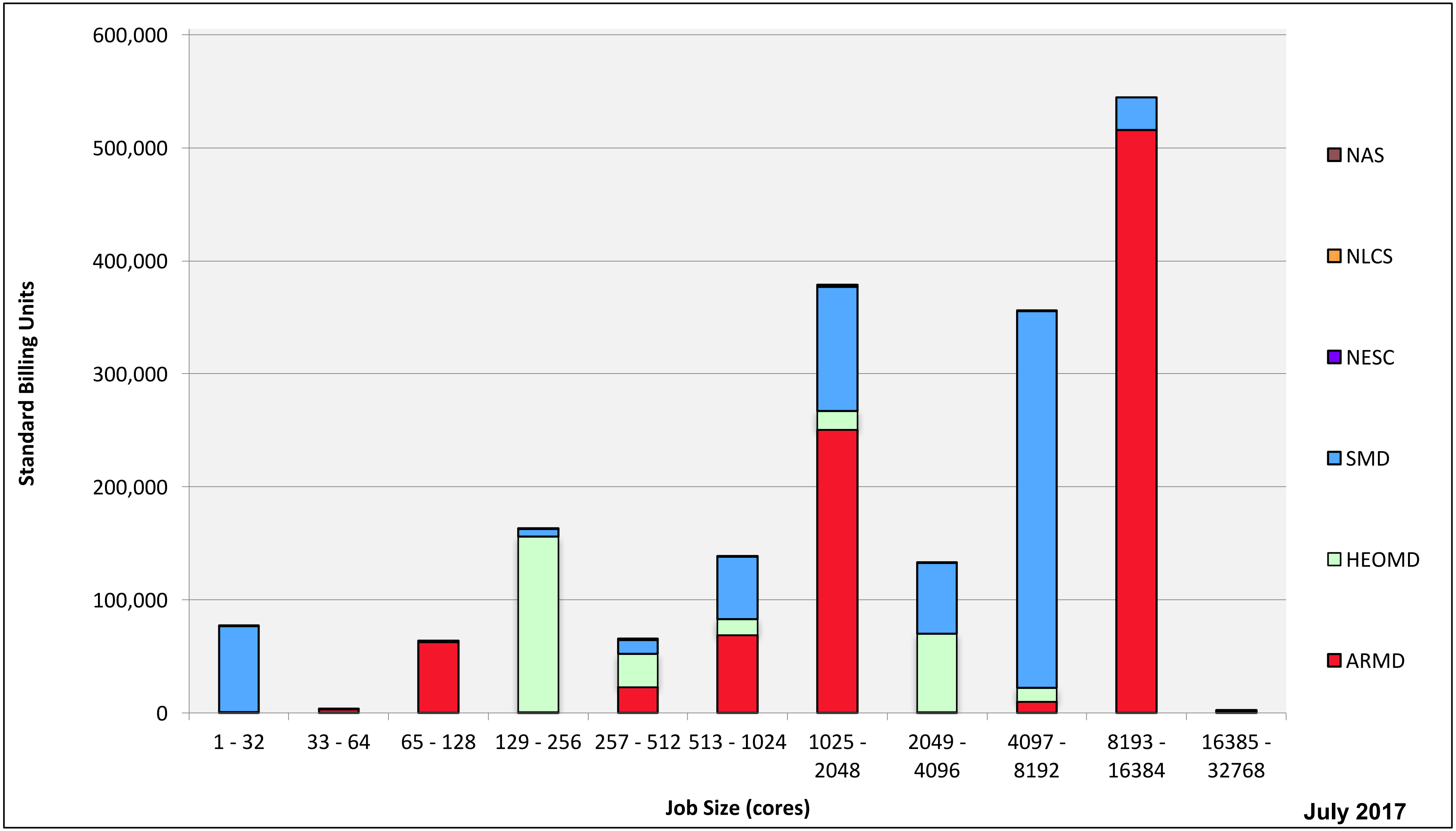
Electra: Devel Queue Utilization



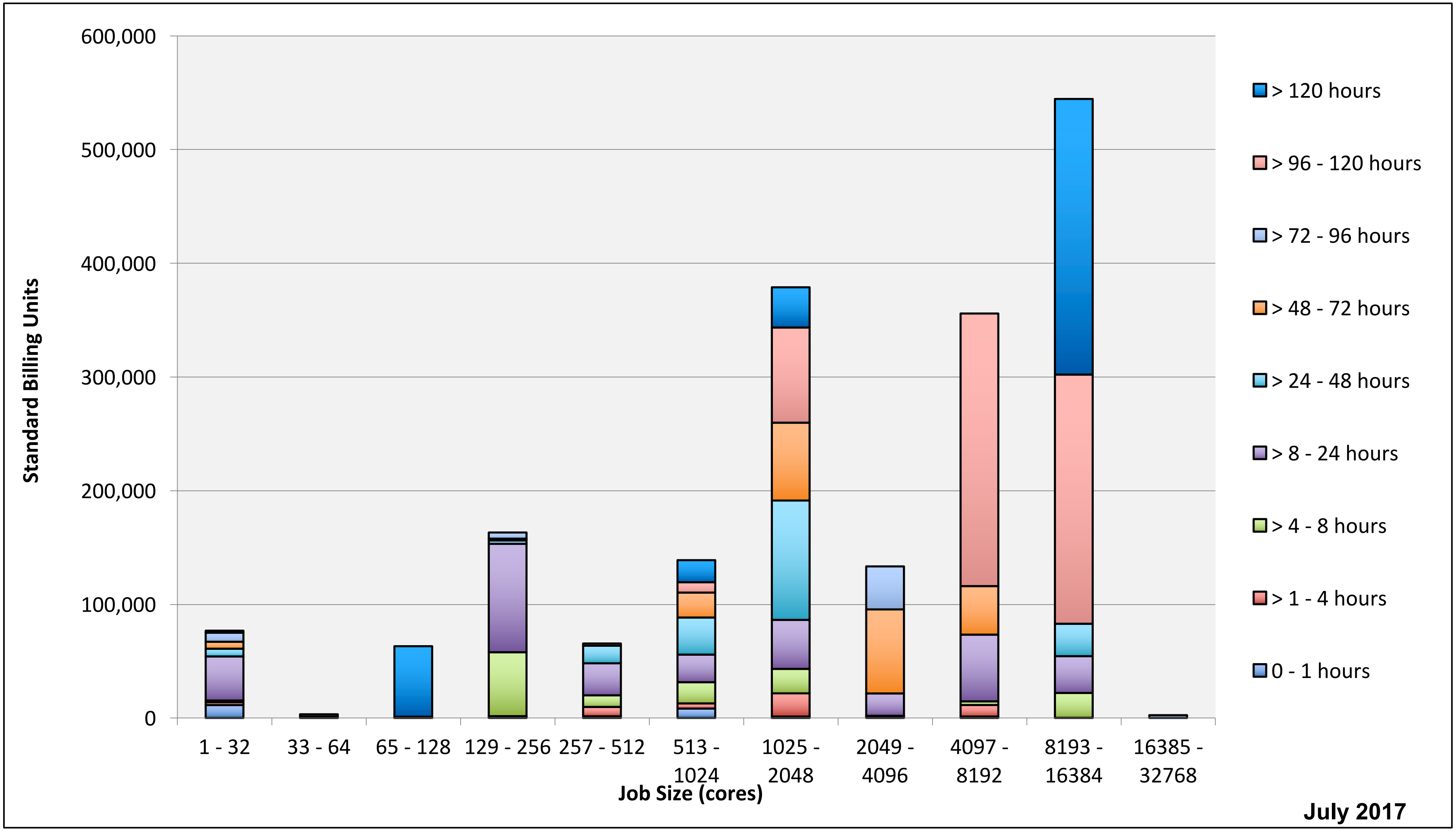
Electra:
Monthly Utilization by Job Length



Electra: Monthly Utilization by Size and Mission



Electra: Monthly Utilization by Size and Length



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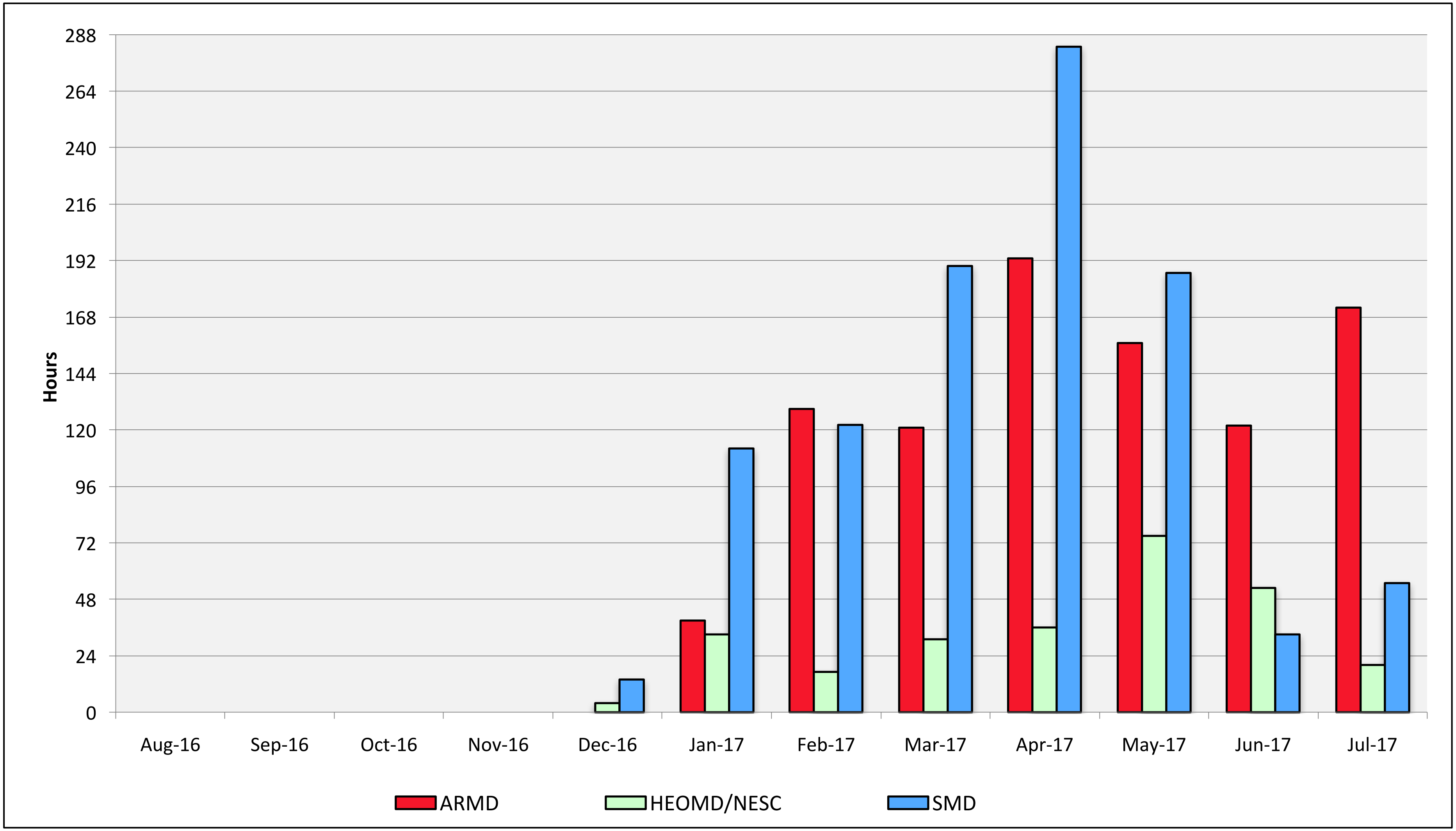
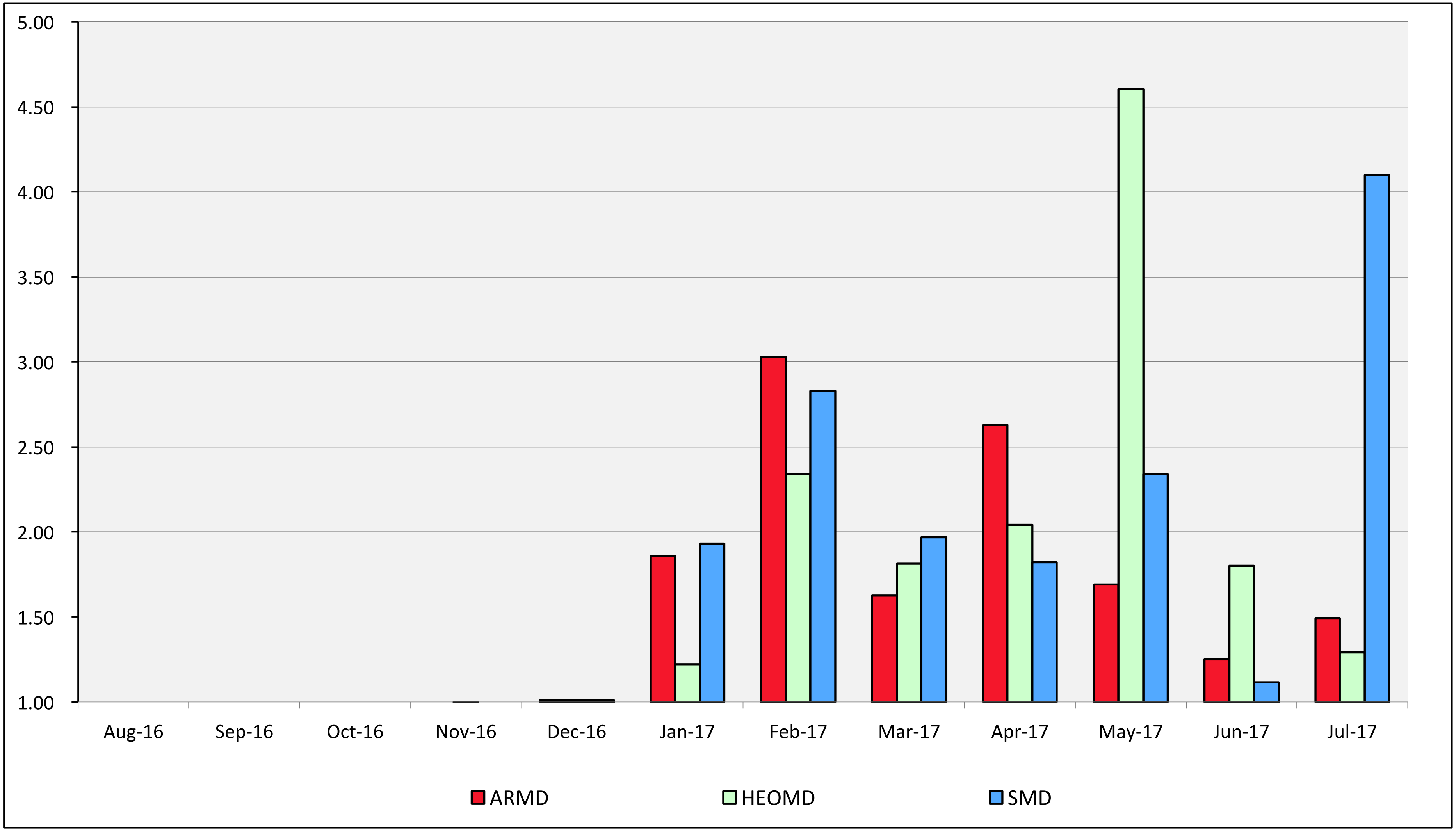
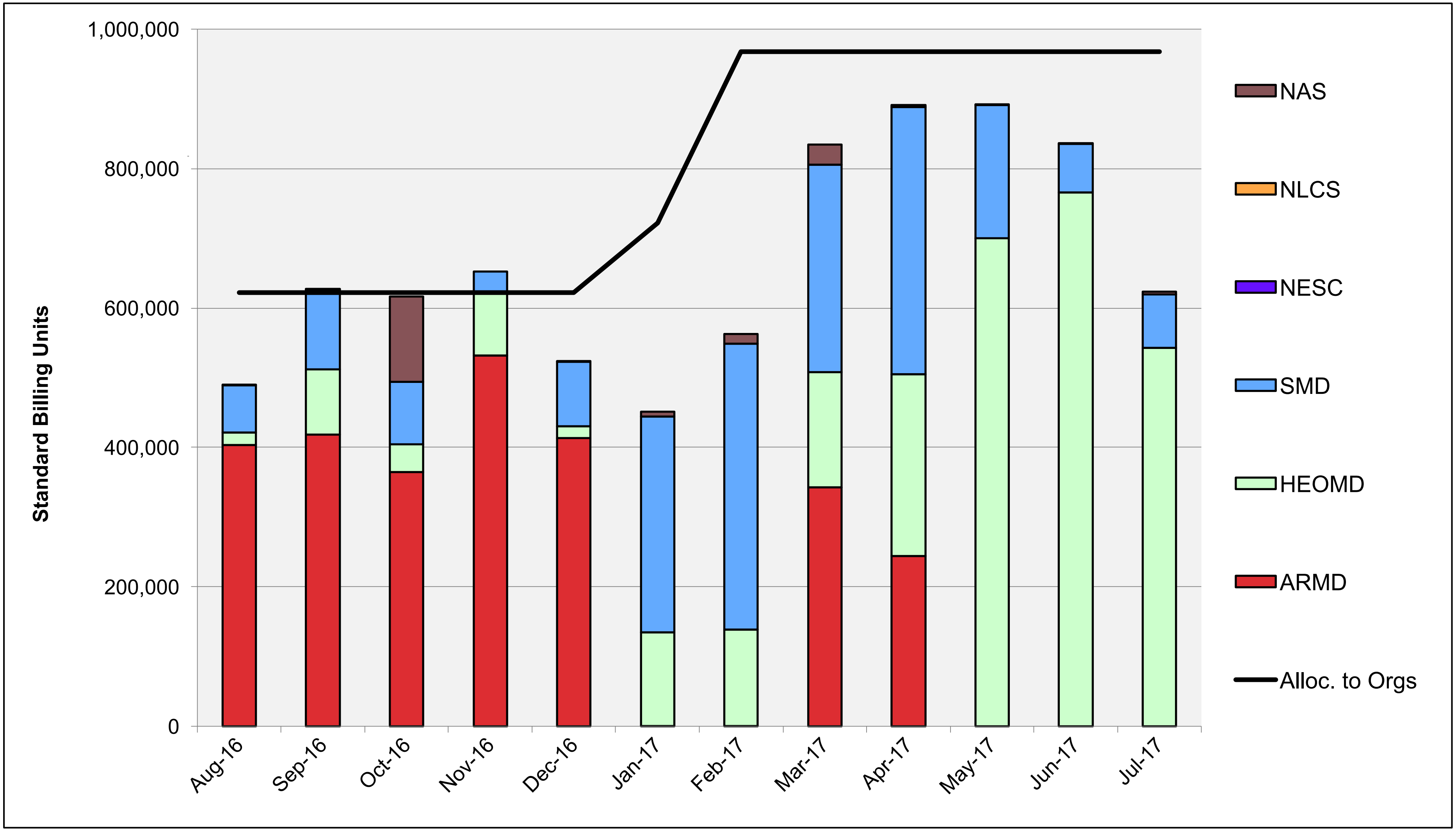


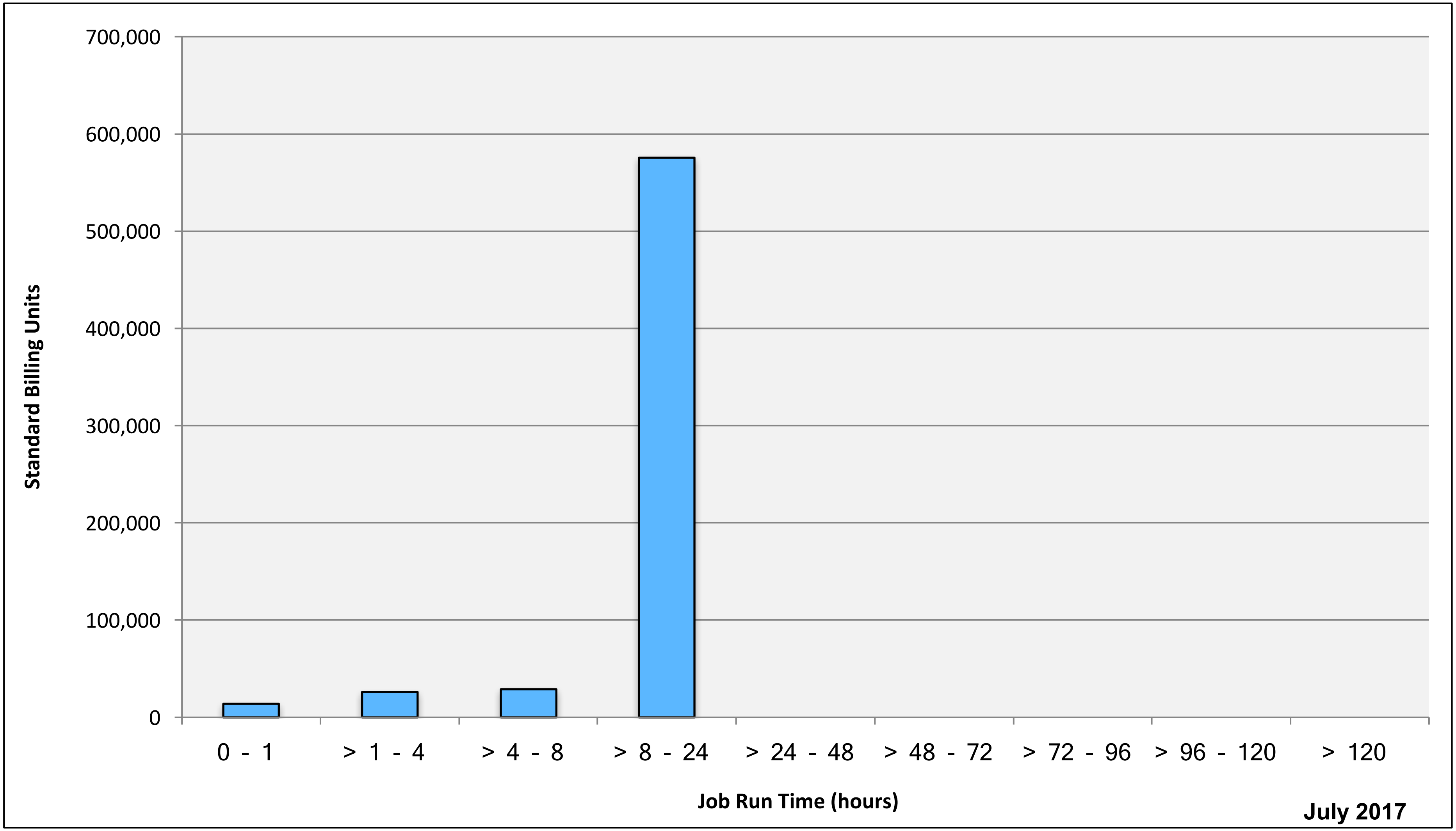
Electra: Average Expansion Factor



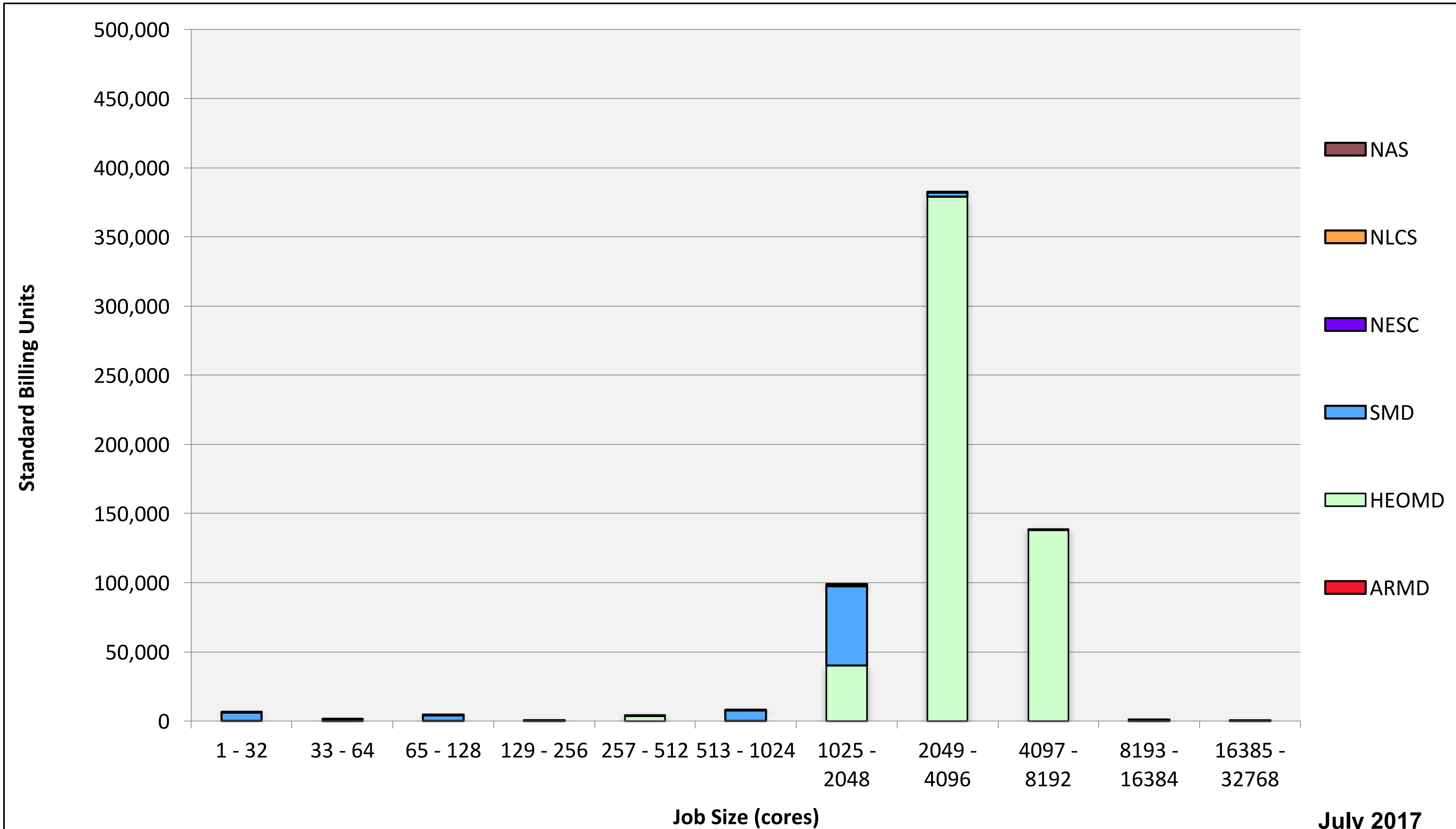
Merope: SBUs Reported, Normalized to 30-Day Month



Merope: Monthly Utilization by Job Length



Merope: Monthly Utilization by Size and Mission



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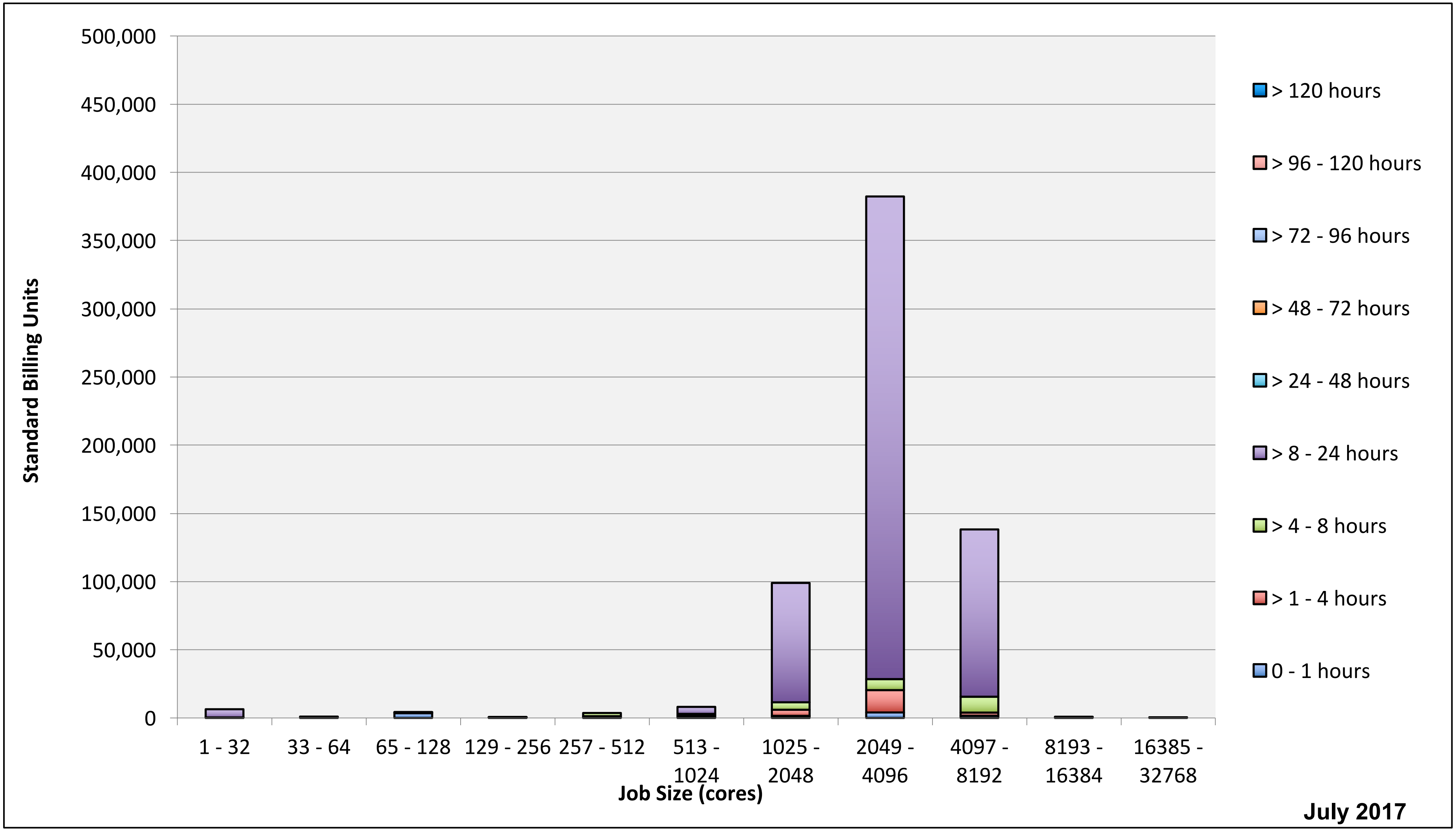
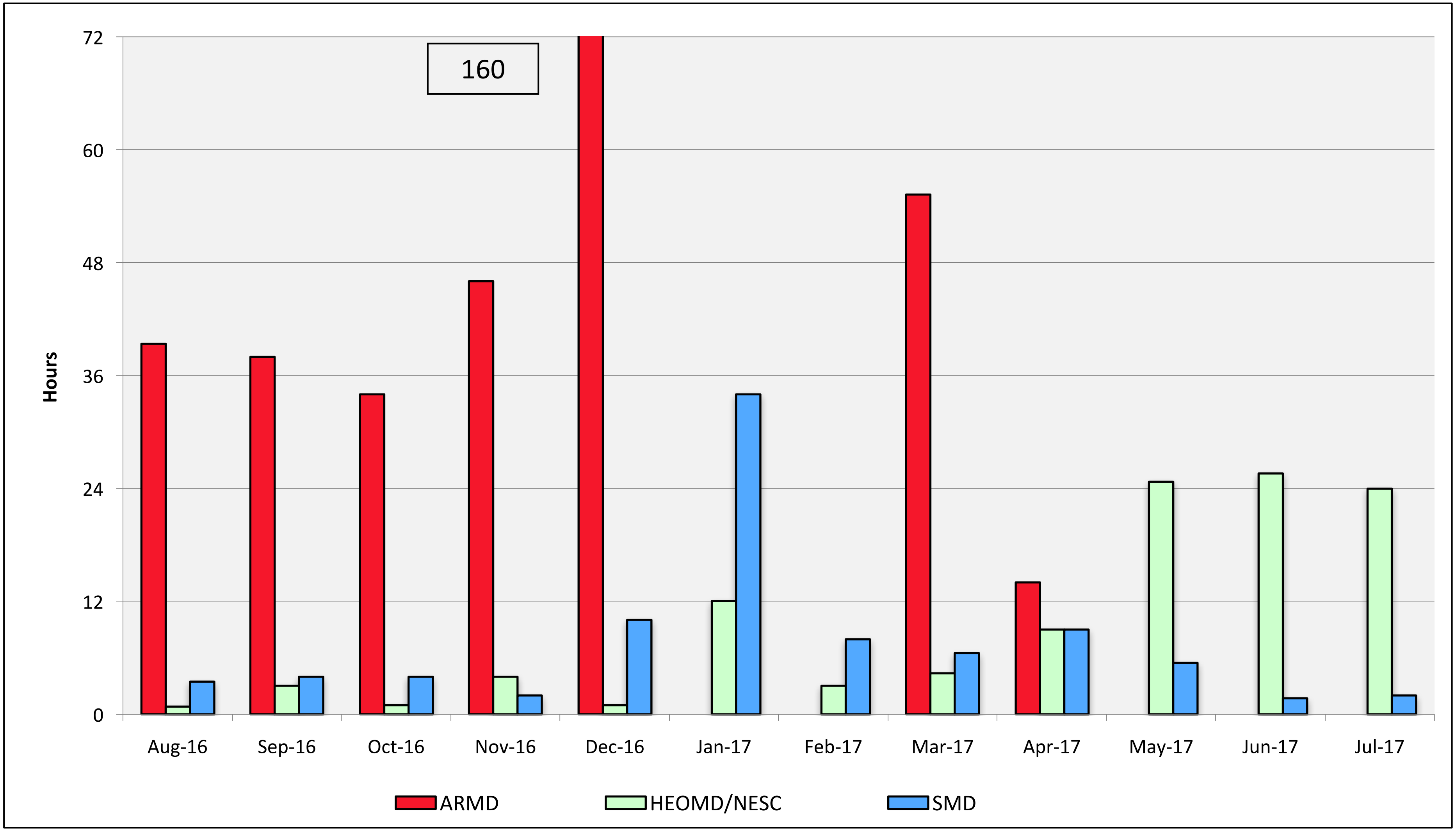
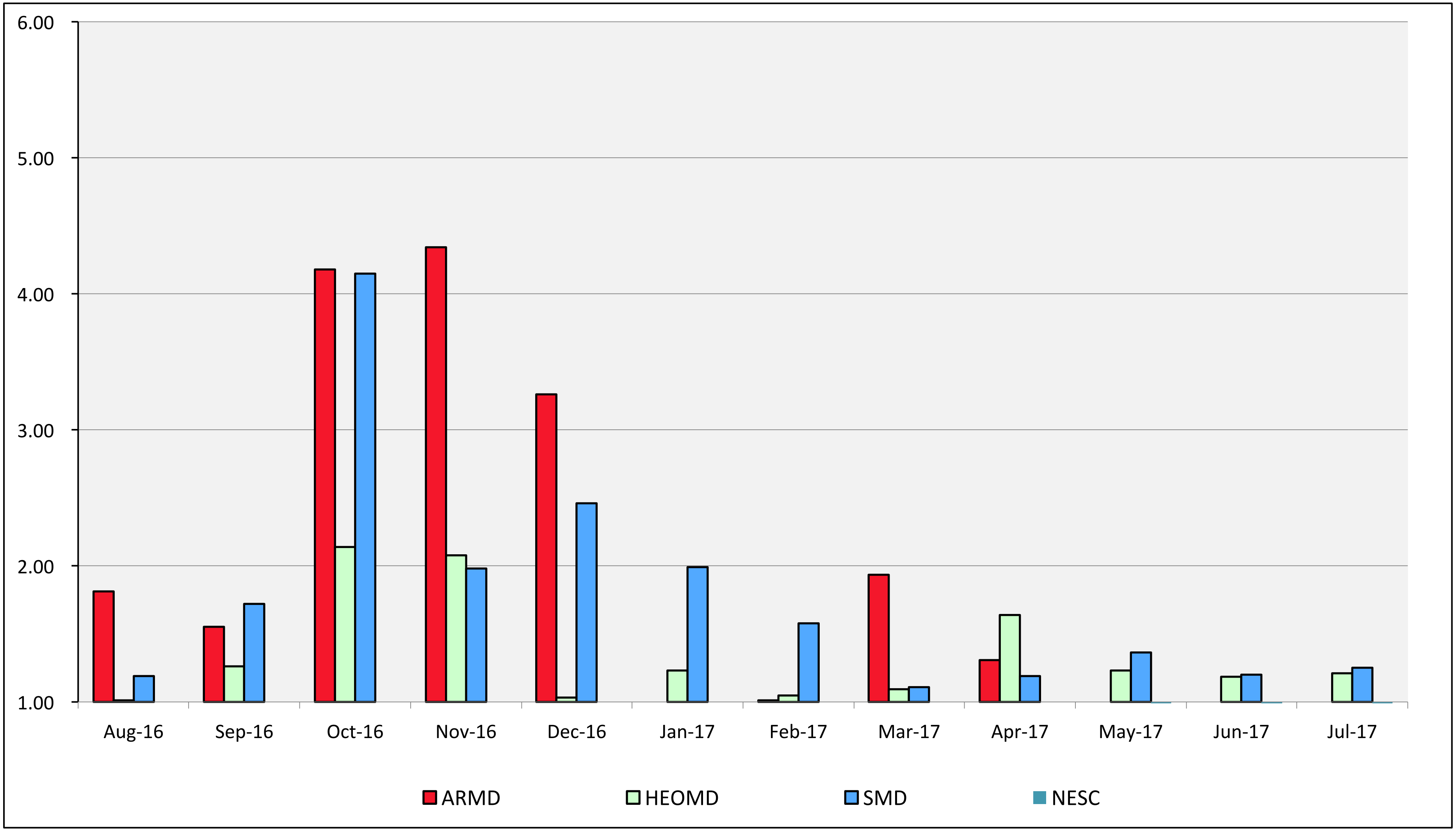


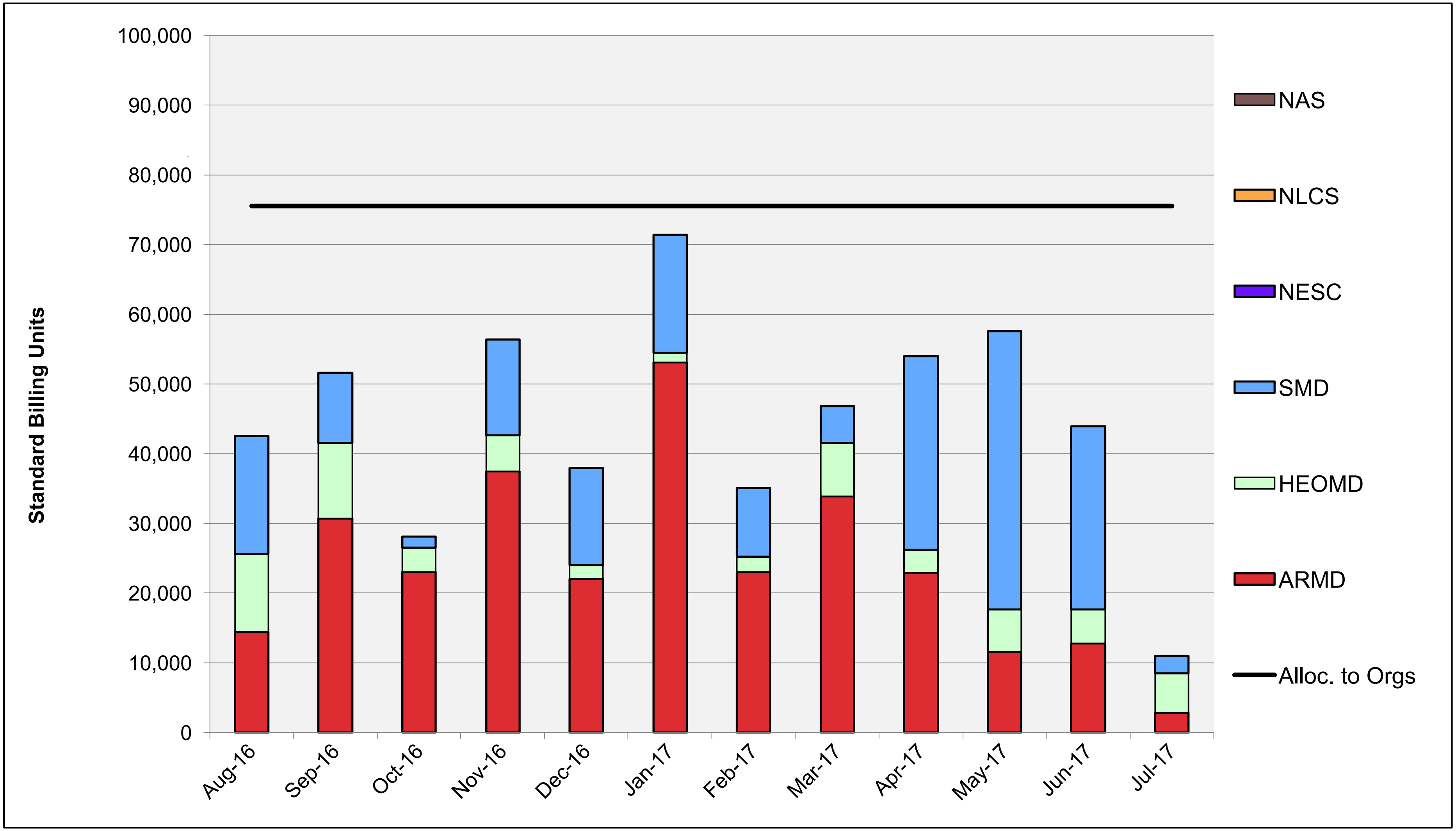
Merope:
Average Time to Clear All Jobs



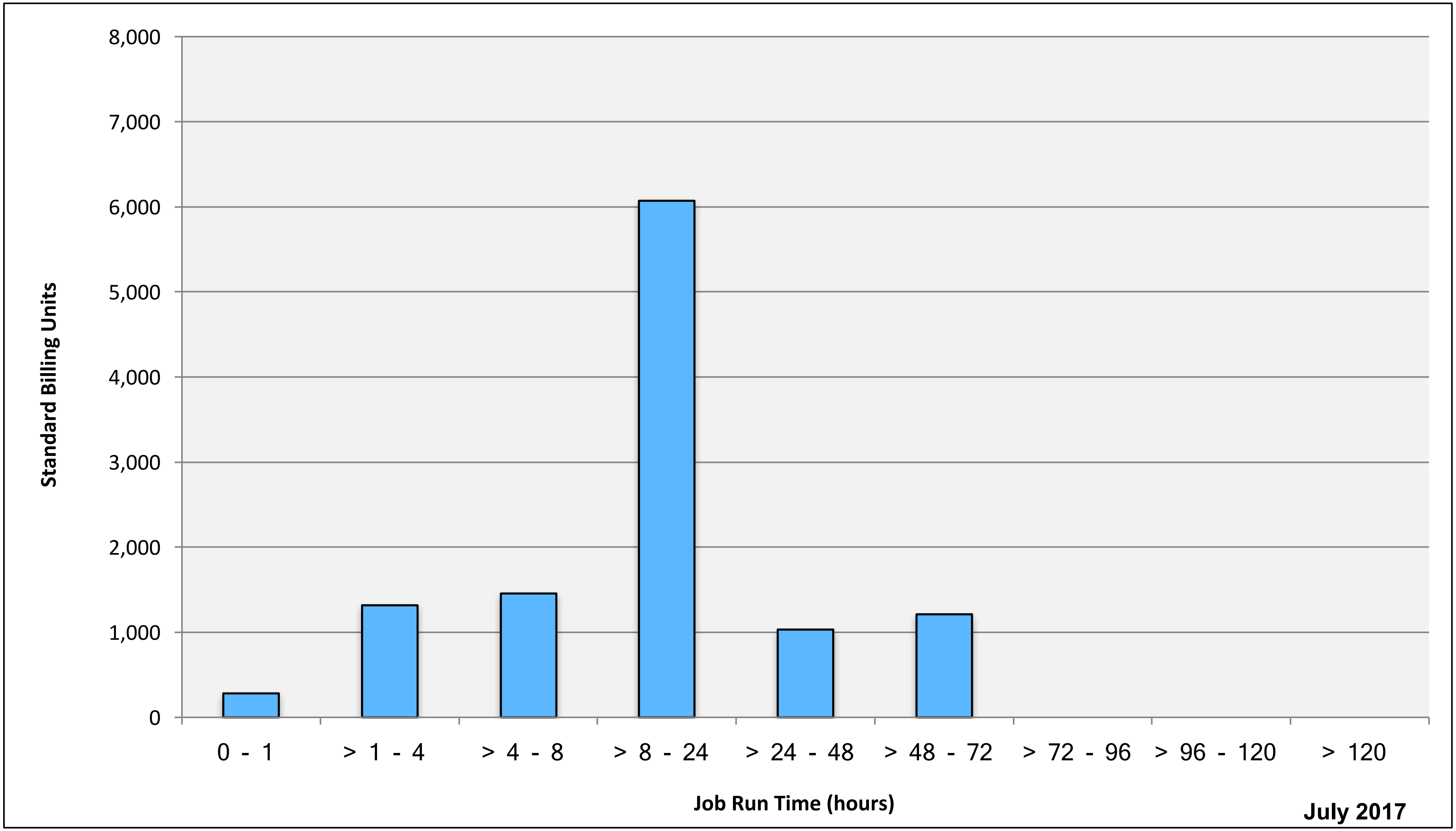
Merope: Average Expansion Factor



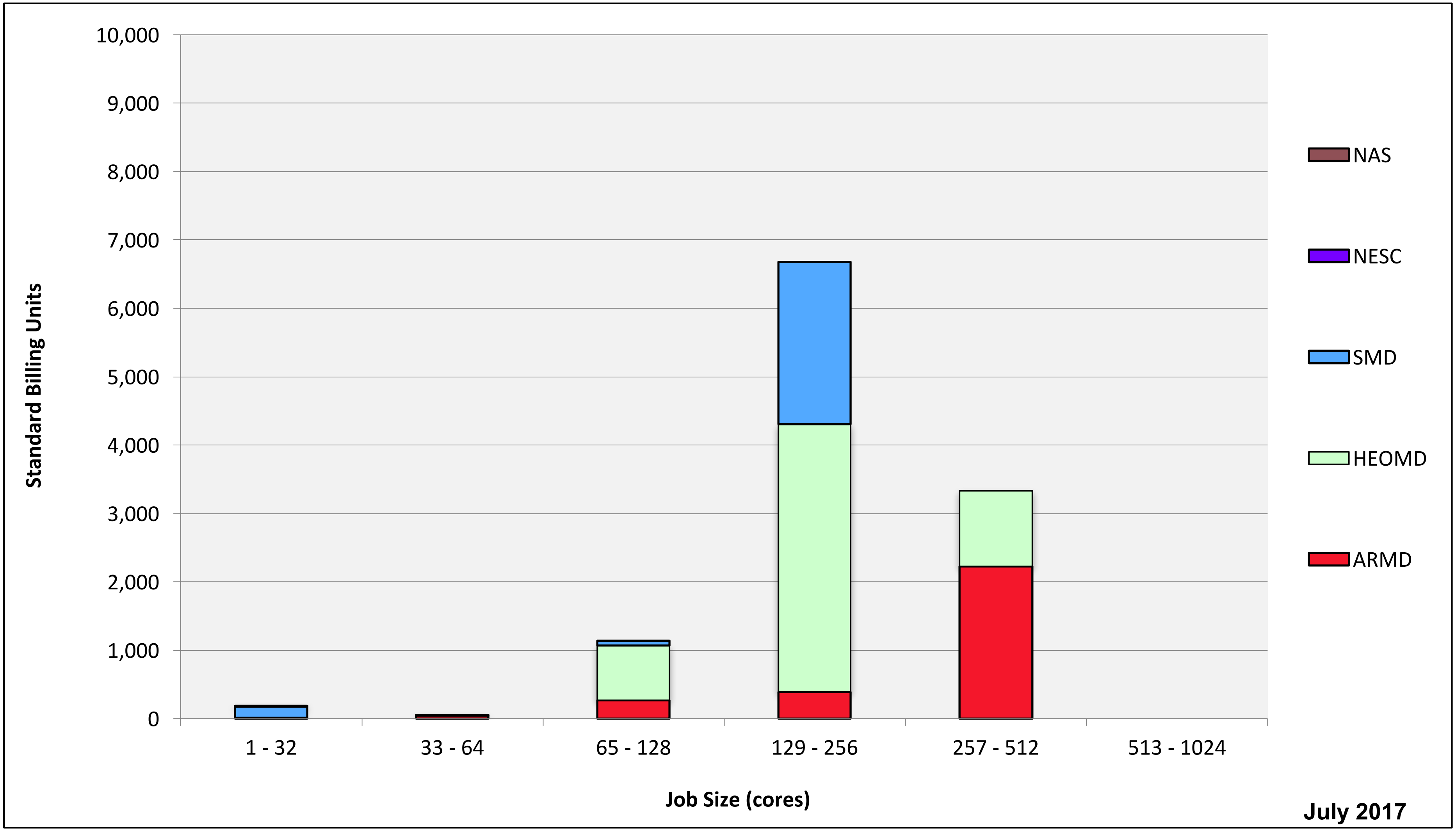
Endeavour: SBUs Reported, Normalized to 30-Day Month



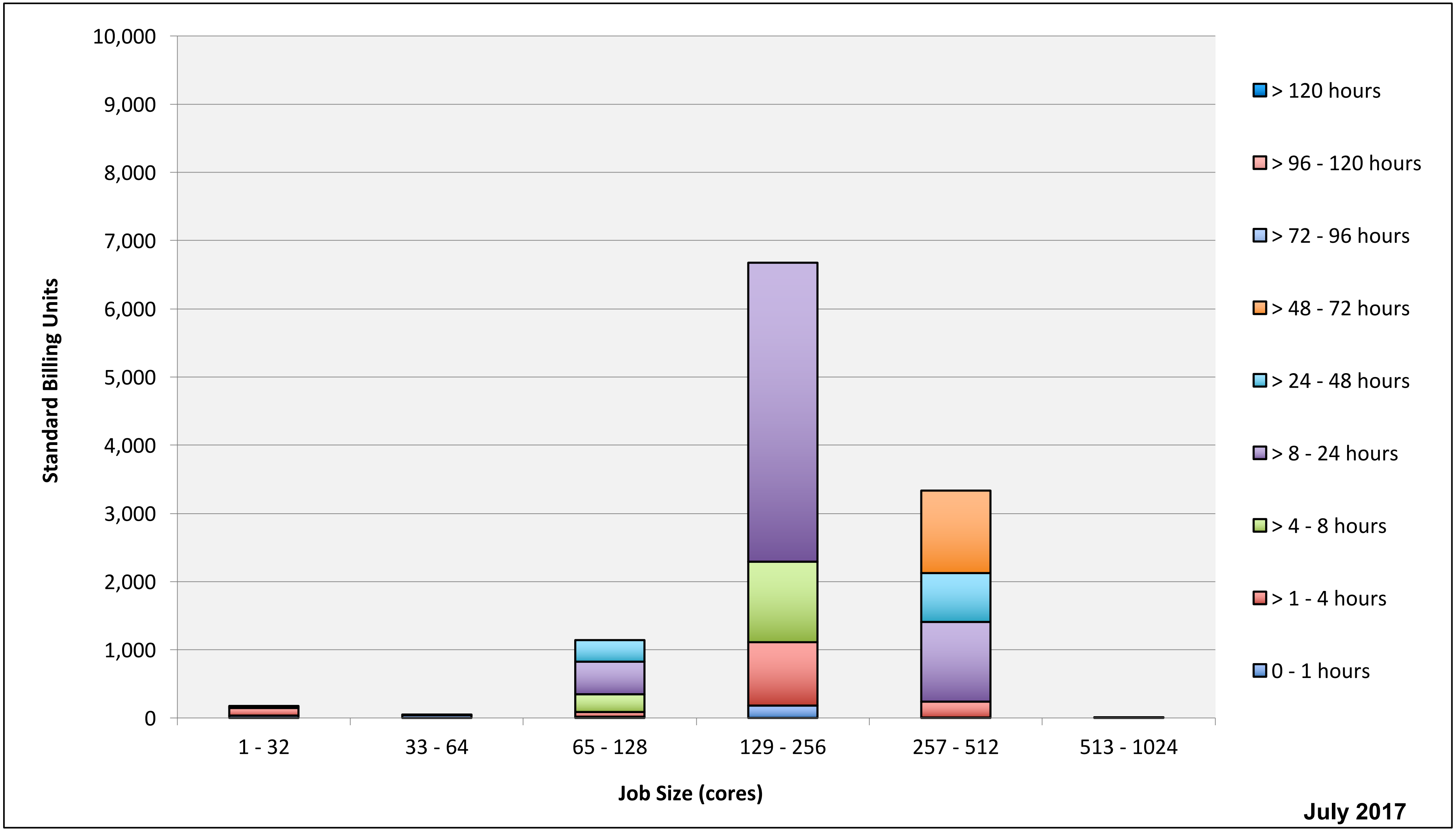
Endeavour:
Monthly Utilization by Job Length



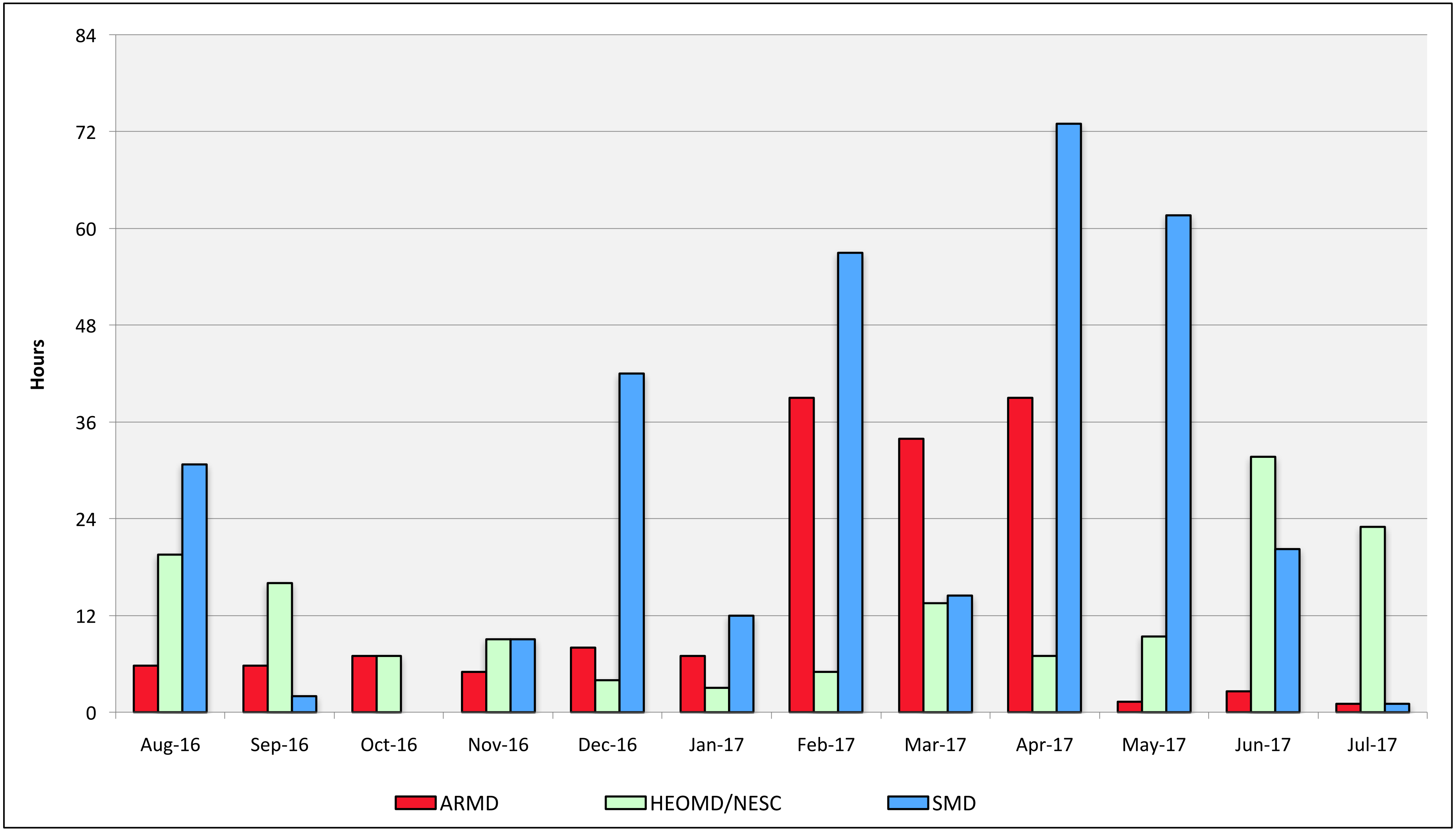
Endeavour: Monthly Utilization by Size and Mission



Endeavour:
Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor